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Computation of Thermally Perfect Properties of Oblique Shock Waves

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Summary

A set of compressible flow relations describing flow properties across oblique shock waves, derived for a thermally perfect, calorically imperfect gas, is applied within the existing thermally perfect gas (TPG) computer code. The relations are based upon a value of c_p expressed as a polynomial function of temperature. The updated code produces tables of compressible flow properties of oblique shock waves, as well as the original properties of normal shock waves and basic isentropic flow, in a format similar to the tables for normal shock waves found in NACA Rep. 1135. The code results are validated in both the calorically perfect and the calorically imperfect, thermally perfect temperature regimes through comparisons with the theoretical methods of NACA Rep. 1135, and with a state-of-the-art computational fluid dynamics code. The advantages of the TPG code for oblique shock wave calculations, as well as for the properties of isentropic flow and normal shock waves, are its ease of use, and its applicability to any type of gas (monatomic, diatomic, triatomic, polyatomic, or any specified mixture thereof).

The TPG code computes properties of oblique shock waves for given shock wave angles, or for given flow deflection (wedge) angles, including both strong and weak shock waves, including the special case of a normal shock. The code also allows calculation of a sequence of shocks where each successive shock wave is dependent upon the flow conditions from the preceding one. Both tabular output and output for plotting and post-processing are available. The user effort required is minimal, consisting of simple answers to 14 interactive questions (or less) per table generated.

Introduction

The traditional computation of one-dimensional (1-D) isentropic compressible flow properties, and properties across normal and oblique shock waves, has been performed with calorically perfect gas equations such as those found in NACA Rep. 1135 (ref. *1*). When the gas of interest is air and all shock waves present are normal to the flow direction, the tables of compressible flow values provided in NACA Rep. 1135 are often used. For shock waves in air that are oblique to the flow direction, NACA Rep. 1135 contains charts of certain flow properties. These tables and charts were generated from the calorically perfect gas equations with a value of 1.40 for the ratio of specific heats γ. The application of these equations, tables, and charts is limited to that range of temperatures for which the calorically perfect gas assumption is valid. However, many aeronautical engineering calculations extend beyond the temperature limits of the calorically perfect gas assumption, and the application of the tables or equations of NACA Rep. 1135 can result in significant errors. These errors can be greatly reduced by the assumption of a thermally perfect, calorically imperfect gas in the development of the compressible flow relations. (For simplicity within this paper, the term *thermally perfect* will be used to denote a thermally perfect, calorically imperfect gas.) Previous papers (references *2* and *3*) described a computer code, and the underlying mathematical formulation, which implements 1-D isentropic compressible flow and normal shock wave relations derived for a thermally perfect gas. The current paper presents an enhanced computer code, and the corresponding mathematical derivation, for the computation of the oblique shock wave relations based upon the assumption of a thermally perfect gas.

A calorically perfect gas is by definition a gas for which the values of specific heat at constant pressure c_p and specific heat at constant volume c_v are constants. Reference *1*, as well as many compressible flow textbooks, derive and summarize calorically perfect compressible flow relations based upon this definition. The accuracy of these equations is only as good as the assumption of a constant c_p (and therefore a constant γ). For any non-monatomic gas, the value of c_p actually varies with temperature and can be approximated as a constant for only a relatively narrow temperature range. As the temperature increases, the c_p value begins to increase appreciably due to the excitation of the vibrational energy of the molecules. For air, this phenomenon begins around 450 to 500 K. The variation of c_p with temperature (and *only* with temperature) continues up to temperatures at which dissociation begins to occur, approximately 1500 K for air. Thus, air is thermally perfect over the range of 450 to 1500 K and application of the calorically perfect relations can result in substantial errors. A similar range can be defined for other gases over which the gas is calorically imperfect, but still thermally perfect. At yet higher temperatures c_p becomes a function of both temperature and pressure, and the gas is no longer considered thermally perfect.

NACA Rep. 1135 does present one method for computation of the 1-D compressible flow properties of a thermally perfect gas. In this approach, the variation of heat capacity due to the contribution from the vibrational energy mode of the molecule is determined from quantum mechanical considerations by the assumption of a simple harmonic vibrator model of a diatomic molecule (ref. *4*). With this assumption the vibrational contribution to the heat capacity of a diatomic gas takes the form of an exponential equation in terms of static temperature and a single constant Θ. The complete set of thermally perfect compressible flow relations based upon this model is listed in NACA Rep. 1135 "Imperfect Gas Effects." Tables of these thermally perfect gas properties are not provided because each value of total temperature T_t would yield a unique table of gas properties. Instead, NACA Rep. 1135 provides charts of the 1-D thermally perfect air isentropic and normal shock properties normalized by the calorically perfect air values and plotted versus Mach number for select values of total temperature. For oblique shock waves, an even more limited set of charts is presented for shock wave angle σ, downstream Mach number M_2, and pressure coefficient as functions of deflection angle δ for four static temperatures at two total temperatures. This approach can only be applied to diatomic gases (e.g., N_2, O_2, and H_2) because the functional form which describes the variation of heat capacity with temperature accounts only for the harmonic contribution.

Because the imperfect gas method of NACA Rep. 1135 is applicable only to diatomic gases, a different method of computing the 1-D isentropic and normal shock flow properties of a thermally perfect gas was developed and described in references *2* and *3*. The current paper extends that methodology to the computation of flow properties across oblique shock waves. The method utilizes a polynomial curve fit of c_p versus temperature to describe the variation of heat capacity for a gas. The data required to generate this curve fit for a given gas can be found in tabulated form in published sources such as the NBS "Tables of Thermal Properties of Gases" (ref. *5*) and the "JANAF Thermochemical Tables" (ref. *6*). Actual coefficients for specific types of polynomial curve fits are also published in NASP TM 1107 (ref. *7*), NASA SP-3001 (ref. *8*), and NASA TP-3287 (ref. *9*). Use of these curve fits based upon tables of standard thermodynamic properties of gases enables the application of this method to any type of gas: monatomic, diatomic, and polyatomic (e.g., H_2O, CO_2, and CF_4) gases or mixtures thereof, provided a data set of c_p versus temperature exists for the individual gas(es) of interest.

In this report, a set of thermally perfect gas equations, derived for the specific heat as a polynomial function of temperature, is applied to the calculation of flow properties across oblique shock waves. This set of equations was coded into a previously developed computer program referred to as the Thermally Perfect Gas (TPG) code. The new oblique shock wave capability was added as an optional output to the isentropic flow and normal shock wave tables of the original code. All of the output tables of the TPG code are structured to resemble the tables of compressible flow properties that appear in NACA Rep. 1135, but can be computed for arbitrary gases at arbitrary Mach numbers and/or static temperatures, for given total temperatures. All properties are output in tabular form, thus eliminating the need for graphical interpolation from charts. As in the original TPG code, the biggest advantage is the validity in the thermally perfect temperature regime as well as in the calorically perfect regime, and its applicability to any type of gas (monatomic, diatomic, triatomic, polyatomic, or any specified mixture thereof). The code serves the function of the tables and charts of NACA Rep. 1135 for any gas species or mixture of species, and significantly increases the range of valid temperature application due to its thermally perfect analysis.

Nomenclature

Symbols:

a	speed of sound
A	cross-sectional area of stream tube or channel
A_j	coefficients of polynomial curve fit for c_p/R of individual species; and for c_p of mixture, equation (3)
c_p	specific heat at constant pressure
c_v	specific heat at constant volume, $c_p - R$
M	Mach number, V/a
p	pressure
q	dynamic pressure, $\frac{\rho V^2}{2}$
R	specific gas constant
T	temperature
u	velocity component normal to the shock wave
V	flow velocity
w	velocity component tangential to the shock wave
Y	mass fraction
z	lateral coordinate to upstream flow, measured from wedge leading edge
γ	ratio of specific heats, c_p/c_v
δ	flow deflection angle; 2-D wedge half-angle
Θ	molecular vibrational energy constant, references *1* and *4*
μ	characteristic Mach angle
ρ	mass density
σ	shock wave angle relative to the upstream flow direction

Subscripts:

1	upstream flow reference point; e.g., upstream of a shock wave
2	downstream flow reference point; e.g., downstream of a shock wave
i	i^{th} component gas species of mixture
j	j^{th} coefficient of polynomial curve fit for c_p
$jmax$	maximum j value
lim	limiting conditions for oblique shock waves
max	maximum value
mix	gas mixture
n	total number of gas species that comprise a gas mixture
$perf$	calorically perfect
$therm$	thermally perfect
t	total (stagnation) conditions

Abbreviations:

1-D	one-dimensional
2-D	two-dimensional
CFD	computational fluid dynamics
CPG	calorically perfect gas
cpu	(computer) central processing unit
GASP	General Aerodynamic Simulation Program
NACA	National Advisory Committee for Aeronautics
NASP	National Aero-Space Plane
TPG	thermally perfect gas

Derivation of Oblique Shock Relations

Polynomial Curve Fit for c_p

The selection of a suitable curve fit function for c_p is the starting point for the development of thermally perfect compressible flow relations. The form chosen for the TPG code was the eight-term, fifth-order polynomial expression given below, in which the value of c_p has been nondimensionalized by the specific gas constant.

$$\frac{c_p}{R} = A_1\left(\frac{1}{T^2}\right) + A_2\left(\frac{1}{T}\right) + A_3 + A_4(T) + A_5(T^2) + A_6(T^3) + A_7(T^4) + A_8(T^5) \qquad (1)$$

For a given temperature range, A_1 to A_8 are the coefficients of the curve fit. This is the functional form for c_p of NASP TM-1107 (ref. *7*), which provides values of A_1 to A_8 for 15 different gas species. NASA SP-3001 (ref. *8*) provides similar c_p curve fit coefficient data (A_3 through A_7) for over 200 individual gas species for a five-term, fourth-order polynomial fit equation. NASA TP 3287 (ref. *9*) provides additional c_p curve fit coefficient data for 50 reference elements for both a five-term (A_3-A_7) and a seven-term (A_1-A_7) fourth-order polynomial fit equation. Equation (1) is valid for each of these curve fit data sets, with appropriate coefficients set to zero. These definitions are typically multi-segmented curve fits defined over contiguous temperature ranges so that the c_p definition is continuous. Thus, for a given species there are typically two or more sets of coefficients, each valid over a given subset of the entire temperature range.

The polynomial curve fit definitions provided in refs. *7*, *8*, and *9* are defined to be valid over specific temperature ranges. Beyond those ranges the accuracy of the data fit may degrade rapidly. All algorithms based upon these data fits should note any calculations at temperatures outside of the stated temperature ranges.

Different algebraic expressions for c_p/R could be exchanged for that of equation (1) within the TPG code. The form of equation (1) was selected in the current work because of its ease of implementation, and the wealth of already available data from references *7*, *8*, and *9*. The only requirements are that closed-form solutions to both $\int c_p dT$ and $\int (c_p/T) dT$ must be known. These requirements are explained in more detail in reference *2*.

Mixture Properties

The TPG code can be used to compute the thermally perfect gas properties for not only individual gas species but also for mixtures of individual gas species (e.g., air). This capability is achieved within the code by calculating the variation of the heat capacity for the specified gas mixture. The mixture c_p is

$$c_{p_{mix}} = \sum_{i=1}^{n} Y_i c_{p_i} \qquad (2)$$

where Y_i is the mass fraction of the i^{th} gas species. The value of c_{p_i} is determined from equation (1) for each component species. This is actually implemented in the code by combining like terms of the polynomials for each individual gas species; that is

$$c_{p_{mix}} = \sum_{j=1}^{jmax} A_{j_{mix}} T^{j-3} \qquad (3)$$

where

$$A_{j_{mix}} = \sum_{i=1}^{n} Y_i R_i A_{j_i} \text{, for j=1, jmax} \qquad (4)$$

With a known curve fit expression for c_p of the gas mixture, the value of γ for a given temperature can be directly computed, as can mixture properties of gas constant and molecular weight. See references *2* and *3* for additional details regarding the derivation of the 1-D isentropic relations and the normal shock relations from these properties.

Oblique Shock Relations

Figure 1 illustrates the geometric relationships associated with a shock wave at an arbitrary shock angle σ relative to the upstream flow direction. These relationships can be expressed as

$$\tan\sigma = \frac{u_1}{w} \qquad (5)$$

and

$$\tan(\sigma-\delta) = \frac{u_2}{w} \qquad (6)$$

where u_1 and u_2 are the upstream and downstream velocity components normal to the shock, and w=w_1=w_2 is the tangential velocity component which is conserved across the shock. Since only the normal component of velocity changes across the shock, the flow is turned through an angle δ. Solving equations (5) and (6) for w, a single equation can be written:

$$\frac{\tan(\sigma-\delta)}{\tan\sigma} = \frac{u_2}{u_1} \qquad (7)$$

The normal velocity components can be expressed as

$$u_1 = V_1\sin\sigma \qquad (8)$$

and

$$u_2 = V_2\sin(\sigma-\delta) \qquad (9)$$

Thus, equation (7) can be rewritten as

$$\frac{\tan(\sigma-\delta)}{\tan\sigma} = \frac{V_2\sin(\sigma-\delta)}{V_1\sin\sigma}\ , \qquad (10)$$

a function of shock angle σ, deflection angle δ, and the upstream and downstream velocities V_1 and V_2.

The continuity and momentum equations for 1-D flow across a shock wave in a shock-fixed coordinate system (a *stationary* shock) are given as follows

$$\rho_1 u_1 = \rho_2 u_2 \qquad (11)$$

$$p_1 + \rho_1 u_1^2 = p_2 + \rho_2 u_2^2 \qquad (12)$$

Dividing the momentum equation by the continuity equation gives

$$\frac{p_1}{\rho_1 u_1} + u_1 = \frac{p_2}{\rho_2 u_2} + u_2 \qquad (13)$$

Using the ideal gas law ($p = \rho RT$), equation (13) can be written in terms of only temperature and normal velocity as

$$\frac{RT_1}{u_1} + u_1 = \frac{RT_2}{u_2} + u_2 \qquad (14)$$

Substituting for u_1 and u_2 with equations (8) and (9), equation (14) becomes

$$\frac{RT_1}{V_1\sin\sigma} + V_1\sin\sigma = \frac{RT_2}{V_2\sin(\sigma-\delta)} + V_2\sin(\sigma-\delta)\ , \qquad (15)$$

a function of shock angle σ, deflection angle δ, the upstream and downstream velocities V_1 and V_2, and the upstream and downstream static temperatures T_1 and T_2. However, as derived in reference *2*, the velocity may be expressed as a function of temperature

$$V^2 = 2\int_T^{T_t} c_p dT \qquad (16)$$

at any point in the flow field, whether upstream or downstream of the shock. Thus, the dependencies on velocity in equations (10) and (15) can actually be expressed as dependencies on temperature.

Assuming all upstream flow conditions are known (state *1*), and substituting equation (16) for V_1 and V_2, equations (10) and (15) represent a set of two nonlinear equations for three unknowns: σ, δ, and T_2. Given any one of these variables, the other two may be found numerically by means of Newton iteration. (Appendix A provides additional details regarding implementation of this Newton algorithm within the TPG code.) If the shock angle σ is known, the tangential velocity component is

$$w = w_1 = w_2 = V_1\cos\sigma \qquad (17)$$

Thus, the downstream normal velocity u_2 can be defined as

$$u_2^2 = V_2^2 - w^2 = 2\int_{T_2}^{T_t} c_p dT - w^2, \qquad (18)$$

a function of T_2 only, instead of both T_2 and δ as in equation (9). Thus, instead of equation (15), equation (14) reduces to a function of T_2 only and can be solved independently of equation (10). For the case of known deflection angle δ, equations (10) and (15) must be solved simultaneously for T_2 and σ.

Once the primary variables of temperature T_2, σ, and δ are known, all other flow quantities may be computed.

$$\gamma_2 = \frac{c_{p_2}}{c_{p_2} - R} \tag{19}$$

$$a_2^2 = \gamma_2 R T_2 \tag{20}$$

$$M_2 = V_2 / a_2 \tag{21}$$

where V_2 is known from equation (16).

Pressure and density downstream of the shock wave can be calculated by the normal shock wave relations derived in reference *2*, noting that all velocity terms (including Mach number) are defined normal to the shock. That is,

$$\frac{p_2}{p_1} = 1 + \gamma_1 (M_1 \sin\sigma)^2 \left(1 - \frac{u_2}{u_1}\right) \tag{22}$$

$$\frac{\rho_2}{\rho_1} = \frac{u_1}{u_2} \tag{23}$$

The values of total pressure loss $p_{t,2}/p_{t,1}$ and the ratio of upstream-static to downstream-total pressure $p_1/p_{t,2}$ can then be calculated from combinations of static and total pressure ratios. See reference *2* for further detail.

Figure 2 illustrates the relationships between M_1, σ, and δ for air at a sample T_t. The figure shows that, for a given M_1 and δ, two solutions exist for σ, corresponding to what are commonly called 'weak' and 'strong' shock waves. A maximum flow deflection angle δ_{max} exists for any M_1, defined as the point at which the weak and strong shock solutions are identical. Strong shock waves always result in subsonic downstream Mach numbers and have shock wave angles approaching 90°. Weak shock waves are those for which the corresponding wave angle σ is less than that at which δ_{max} occurs, and usually result in supersonic downstream Mach numbers, except as σ approaches $\sigma(\delta_{max})$.

Oblique shock waves can only exist at Mach numbers above a limiting case, i.e., $M_1 > M_{1,lim}$. For a given σ, the limiting case occurs at $\mu=\sigma$, where the Mach angle μ is defined by

$$\sin\mu = \frac{1}{M_1} \tag{24}$$

At these conditions the shock strength and δ reduce to zero. Obviously, μ is only defined for M_1 greater than, or equal to, 1, and thus, oblique shocks can not exist at subsonic upstream conditions. For sonic upstream conditions $M_1=M_{1,lim}=1.0$, $\sigma_{\text{lim}}=90°$ and $\delta_{\text{lim}}=0°$.

For a given δ, the limiting case $M_{1,lim}$ corresponds to the Mach number for which $\delta=\delta_{max}$. From a physical perspective, this limit is the minimum Mach number at which an attached shock wave can occur at the leading edge of a wedge. Below $M_{1,lim}$ the flow results in a detached strong shock wave standing a finite distance upstream of the wedge leading edge, and the flow approaching the point of turning is subsonic, not supersonic.

Oblique Shock Code Description

An interactive FORTRAN computer code, herein referred to as the TPG code, has been written based on the equations described herein and those described in references *2* and *3*. This code delivers a complete table of results within seconds when run on a computer workstation or personal computer. The purpose and primary output of the code is the creation of tables of compressible flow properties for a thermally perfect gas or mixture of gases (styled after those found in NACA Rep. 1135). In addition to the isentropic flow and normal shock wave properties of the previous version of TPG, the latest release of the TPG code (version 3.1) computes properties across oblique shock waves, given either the shock wave angle σ or the flow deflection angle δ. Tabular entries may be based upon constant increments of Mach number, or constant decrements of static temperature from the total temperature. Such tables are presented in NACA Rep. 1135 only for isentropic flow and normal shock waves, and only for calorically perfect air (γ=1.40) at constant increments of Mach number. Only charts (no tables) are presented therein for oblique shock wave properties. As in previous versions (see references *2* and *3*), the utility of the TPG code is its capability to generate tables of compressible flow properties of any gas, or mixture of gases, for any total conditions over any specified range of Mach numbers or static temperatures ($T<T_t$, of course). Thus, the code recognizes that the properties of thermally perfect gases vary with both total temperature T_t and static temperature T, rather than with only the ratio of T/T_t.

In this section, the newest segments of the TPG code, Version 3.1, are described, code execution procedures are outlined, and examples are provided of user-supplied inputs. Various types of output are also described.

The FORTRAN code consists of a *Main* program, three *include* files, and 18 subroutines, plus a *Block Data* initialization routine. The subroutines are grouped according to purpose within nine files and are called as needed from various locations within the *Main* program as well as from other subroutines. Version 3 was modularized to a greater extent than Version 2 to simplify and shorten the *Main* program, and to facilitate the internal documentation of the source code. Table 1 summarizes the files and subroutines which comprise the TPG code. A Unix Makefile has been developed for compilation of the code and creation of an executable. Defaults are provided for all inputs and a complete execution requires, at a minimum, answering each interactive prompt with a comma, followed by a "*carriage return*." Such a minimal execution generates a single output file containing a table of the basic isentropic flow properties for the standard composition of air. More extensive tables (such as for oblique shock waves), tables for other gas mixtures, or files for post-processing require specific inputs, which will be described in the following subsection. Some computer platforms require *all* character variable inputs to be delineated by quotes, while other computers only require quotes for strings which include blank spaces. All platforms on which the TPG code has been tested to-date do accept quotes. Therefore, for simplicity within this report, all character variable inputs are shown within quotes. This is the recommended procedure for computer platform independence.

Table 1: TPG Version 3.1 files and subroutines

Files	Subroutines
TPG.f	*Main* program
Version.h	*Include* code version identifier
params.h	*Include* parameters
dimens.h	*Include* common blocks
initd.f	Subroutines *initd* and *Block Data*
mixture.f	Subroutine *mixture*
trangej.f	Subroutine *trangej*
floprop.f	Subroutines *isntrop* and *shokwav*
cpsubs.f	Subroutines *cpeval*, *cpNtgra*, and *cptNtgr*
ntgrat.f	Subroutines *intCp* and *intCpT*
citer.f	Subroutines *Cosigm* and *Codelt*
titer.f	Subroutines *t1iter*, *Todelt*, *Tosigm*, *sta2lim*, and *parabt*
postout.f	Subroutine *postout*

The *Main* Program

The *Main* program handles the interactive input and tabular output, and serves as a driver for the subroutines which perform the actual computation of the mixture properties and flow variables. The following paragraphs describe the interactive inputs for using the code. Later subsections describe the subroutines called from *Main* (see table 1), and provide some details on their algorithms and coding.

The first part of the *Main* program contains the interactive inquiries and responses which specify the gas components, the desired total temperature, and the desired outputs and output formats. A typical example of code execution is shown in Table 2 in which the user responses are italicized (and numbered in the left margin). A response of a comma indicates acceptance of a program default. Each user response is followed by a *carriage return* (shown as ↵).

The first response required *[1]* is an identifier character string (an ID), or symbol name, for inclusion within output files. The ID can be a maximum of 70 characters, entered on a single line. A default ID (for air) may be specified by a "comma" or the word 'DEFAULT' (all upper case or all lower case characters), in which case the next three questions, *[2]*-*[4]*, are omitted and defaults are assumed. A particular database file name may be entered as response *[2]*, the prescribed file containing the necessary thermochemical data for the gases of interest. The file name can be 80 characters, maximum, including file path information. The contents of such a database file is described in detail in reference *2*, and is summarized in a later subsection. The code contains the database necessary to define a four species mixture of air; this default is chosen by entering a comma. The gas mixture definition is completed by responses *[3]* and *[4]* in which the number of individual species, and the corresponding mass fractions, are specified. Defaults are shown as part of the program queries, and may always be selected; they initially correspond to the standard composition of air. Regardless of the number of fractions, the code checks to see if the sum of the mass fractions is equal to unity, and if the database contains sufficient information for the requested case. If the mass fractions do not sum to unity (within a small tolerance), the code issues an error message and stops execution. If the sum is within unity plus-or-minus the tolerance, the last species fraction is recomputed such that the total is precisely unity and a warning message is output describing the change. If the database contains insufficient information an error message is output and execution is terminated.

Responses *[1]* and *[2]* are sensitive to the case of the alphabetic characters entered. That is, upper and lowercase alphabetic characters have unique meanings. However, all succeeding inputs are <u>in</u>sensitive to case, and either upper or lowercase responses have the same meaning within the code.

The next inputs define the composition and format of the table(s). The total temperature, response *[5]*, specifies the upper temperature limit (for which the Mach number is zero). Input *[6]* specifies whether the tables are to be in terms of static temperature (T) or Mach (M) number increments. Successive entries in the table(s) may be given at Mach numbers from an initial Mach up to an upper Mach number limit, for constant step sizes of Mach, response *[7]*. Alternatively, if the constant static temperature option is specified in response *[6]*, the table entries are of static temperatures from an initial temperature down to the low temperature limit, for constant step sizes of static temperature, also entered as response *[7]*. The initial values are the total conditions by default. These inputs are separated by commas, and any, or all, may be defaulted simply by entering a comma alone. (See responses *[6]* and *[7]*, for example.)

Response *[8]* specifies which properties are to be included in the table(s). Isentropic flow properties are always included in the table(s), and constitute the default for response *[8]*. The basic table can be expanded to include properties across shock waves through selection of menu options 1, 2 or 3. Oblique shock waves can be specified through either a specific shock wave angle σ, or as the shock wave required to turn the flow through a given angle δ. Normal shocks are a special case of the oblique shock wave with σ=90°. For menu options 2 or 3, response *[9]* is required to specify the appropriate angle in degrees, σ or δ, respectively. Response *[10]* allows the user to choose the desired shock wave type, either 'weak' or 'strong', for the given δ of menu option 3, response *[8]*, and is omitted for all other options. Similarly, responses *[9]* and *[10]* are both omitted for menu options 0 and 1.

The relative positions of the tables of isentropic and shock wave properties are determined by response *[11]* regarding the number of tables (either 1 or 2). The shock wave properties and the isentropic properties may be output in two separate tables cross-referenced by Mach number and static temperature, or in a single, wide-format table (156 characters across). The sepa-

Table 2: Sample TPG v3.1 interactive inputs

```
|   Thermally Perfect Gas Properties Code   |
|              TPG, Version 3.1.0           |
|                                           |
|       NASA  Langley Research Center       |
```

```
              Enter the ID ('character string') for the gas mixture:
                      [default = 4-species Air]
                {enter a comma (,) to accept any default}
[1]           'Sample Combustion Products' ↵
              Enter the name of the Database File for the Species properties:
[2]           'CombProd.data' ↵
              Enter the number of species composing the mixture:  [default = 4]
[3]           6 ↵
              Enter the mass fraction, Y, of all  6 component species
                  in the order of the Database File (sum=1.0):
                [defaults = 0.7553, 0.2314, 0.0129, 0.0004]
                [defaults = 0.0000, 0.0000,
[4]           .1, .6, .2, .0303, .04 ↵
              Enter the Total Temperature (in degrees K):   [default =  400.]
[5]           1500. ↵
              Output the table entries by incremental Temp (K)
               or incremental Mach number? (T/M)
                [default = M]:
[6]           , ↵
              Enter the Initial Mach number, the Mach number Increment,
               and the Upper Mach number Limit:
                   [defaults =    0.,   0.1,   5.0]
[7]           , .2, , ↵
              Enter the appropriate Index from the following Menu:
                      0  :  Isentropic Flow Properties only, ---->  [DEFAULT]
                                or additionally include
                      1  :  Normal Shock Wave Properties,
                      2  :  Oblique Shock Wave Properties, Shock angle given,
                      3  :  Oblique Shock Wave Properties, Deflection given,
[8]           3 ↵
              Enter the Flow Deflection Angle in degrees :   [default = 10.000 degrees]
[9]           , ↵
                Weak or Strong Shock solution: w/s      [default = Weak]
[10]          , ↵
              Enter the number of Tables to be output, 1 or 2 :   [default =   2]
[11]          1 ↵
              Enter the Tabular output location: screen=6, file=9 [default = 9 : TPG.out]
[12]          , ↵
              Do you want to output a TECPLOT file [TPGpost.dat] ? (y/n):   [default = N]
[13]          'y' ↵
              Continue calculation to a succeeding state? (y/n)
                [default = N]:
[14]          , ↵
              STOP: NORMAL
```

rate (second) table of shock wave properties always begins with the lowest Mach number for which a valid solution of the equations exists, that is, $M_{1,lim}$. Succeeding entries are for Mach numbers greater than $M_{1,lim}$. In the single table format, explanatory text is output under the shock property headings when shock property data is not valid.

The table(s) are written to an output file, **TPG.out**, by default since they can be rather extensive. The output file can then be viewed on-line or printed via an appropriate system command. However, if the user desires, the tables can be written to standard output (typically the computer screen), as specified in response *[12]* to the question of tabular output location.

Response *[13]* determines the output of an additional file for data plotting and postprocessing. Because of extensive usage at NASA Langley Research Center, the Tecplot[1] (ref. *10*) code format has been chosen for this file. The basic postprocessor file **TPGpost.dat** contains the same data as that in the **TPG.out** tabular output. The format of this ASCII file, described in reference *10* and in appendix B of reference *2*, could be easily modified to satisfy the input requirements of many different graphics postprocessors. One, two, or three zones of information for all variables and all table entries are included. The first zone includes all subsonic conditions, and always contains, at a minimum, total (stagnation) and sonic entries. The last zone contains all supersonic conditions for which the desired shock wave exists. For oblique shock waves with $M_{1,lim}$ greater than sonic, an intermediate zone is written containing conditions between, and including, sonic and the first shock wave. The second and third zones are omitted if no supersonic conditions are present. The shock wave properties have no physical meaning at subsonic conditions (similarly with supersonic conditions below the limiting Mach number) and are defaulted to a large negative number as a warning flag.

1. Tecplot: trademark of Amtec Engineering, Inc., Bellevue, WA 98009-3633.

Response *[14]* allows the user to compute a succession (or *train*) of shock waves where the upstream conditions of each succeeding shock wave is based upon the downstream conditions of the preceding one. The default response is to end the current set of calculations. An affirmative response *[14]* returns the user to the menu of options, waiting for a new response *[8]*. Thus, the mixture ID, composition, and total temperature are retained, and the table entries are determined by the downstream conditions of the preceding calculation.

Following interactive inputs *[1]*-*[13]*, the database file, if one is requested, is opened, read, and closed. Properties of the gas mixture are computed and the coefficients of the c_p relationship for the mixture are defined (equations (3) and (4)). The **TPG.out** file is opened and header information is written to it stating the gas mixture specifications and the total temperature. The coefficients of the mixture c_p relationship are also listed (equation (4)). A sample header is shown in table 3.

Through calls from the *Main* program to various subroutines (see table 1) the data arrays are initialized, stagnation and sonic conditions are computed, and the isentropic flow properties are computed for each Mach number or static temperature entry in the table, as requested by the user in responses *[6]* and *[7]*. These properties are then output to **TPG.out** unless shock properties are requested in conjunction with the single table format. If shock wave properties are requested (response *[8]*), the code next determines the limiting Mach number and temperature conditions for existence of the shock wave. Beginning with the first entry at a greater Mach number (lower static temperature), the shock wave properties are computed to complete the data set. Tabular output to **TPG.out** is completed and the file is closed. The same information is then output in postprocessor format to the **TPGpost.dat** file.

The default "*N*" ("no") for response *[14]* terminates the calculation. Code execution is completed by closing all files and recording warning summaries of the times the valid temperature ranges were exceeded during the calculations.

These warnings, if any, are related to the database information and are written to an additional file called **Extrap.WARN** for later reference by the user.

Include (or Header) Files

Three files contain statements that are incorporated into the *Main* program and various subroutines via FORTRAN *include* statements at program compilation. The **Version.h** file contains a character variable which specifies the current version number of the computer code. This information is output at the beginning of each interactive execution and to the first lines of the **TPG.out** file.

The **params.h** and **dimens.h** files contain information which determines the amount of computer memory required to execute the TPG code, and, thus, the size of the case which may be specified. The dimensions of the primary arrays within the code as defined below are included in a FORTRAN *parameter* statement in **params.h** and have the following values as released in Version 3.1:

mtrm (=8):	number of polynomial terms which define the relationship for c_p/R,
mspc (=25):	maximum number of gas species allowed,
mcvf (=3):	maximum number of temperature ranges per species allowed and corresponding sets of polynomial coefficients,
mtncr (=10000):	maximum number of computed static temperatures.

All variables assigned to the preceding parameters, except *mtrm*, may be changed to suit particular user requirements. A change in *mtrm* may require coding changes in the subroutines which perform specific calculations using the $c_p(T)/R$ relationships. (See the section "Polynomial Summation and Integration Subroutines" in reference *2* for details on such changes.) The **dimens.h** file specifies *common blocks* containing all of the major arrays that are dependent on the parameters described above.

Mixture and Basic Flow Properties Subroutines

Subroutine *mixture* combines the individual gas species data using the user-specified mass fractions to compute corresponding mixture properties. The database file is opened and read, if needed. The mixture molecular weight and specific gas constant are computed and the mixture polynomial curve fit coefficients are computed according to equation (4). The valid temperature limits of this mixture curve fit are determined from the individual species temperature limits. The lower temperature limit of the mixture is chosen as the greatest minimum temperature of all species with nonzero mass fraction. Similarly, the upper temperature limit of the mixture is chosen as the smallest maximum temperature of all species with nonzero mass fraction.

The *isntrop* subroutine computes the basic properties of isentropic expansion from total (stagnation) conditions for a given static temperature. The *shokwav* subroutine computes the conditions downstream of a shock wave, relative to the upstream conditions from known values of the shock wave angle σ, the flow deflection angle δ, the downstream static temperature T_2, and the downstream velocity V_2. These four fundamental properties are either given as inputs or computed in the oblique shock wave subroutines (*see the following subsection*).

For any known Mach number M the corresponding static temperature T can be determined from the nonlinear relationship

$$2\int_{T}^{T_t} c_p dT = M^2 \gamma R T \tag{25}$$

in which γ is also a function of T. Subroutine *t1iter* performs this function within the TPG code. See reference *2* for additional details regarding this subroutine and algorithm (unchanged from reference *2*).

Oblique Shock Wave Subroutines

As stated previously, equations (10) and (15) are nonlinear functions of three variables (σ, δ, and T_2) which define the relations across an arbitrary oblique shock wave. These equations are solved within the TPG code through Newton iteration algorithms, given one of the two angles σ or δ. Subroutine *Todelt* solves for δ and T_2 given σ, and *Tosigm* solves for σ and T_2 given δ. The downstream velocity component u_2 (and, thus, V_2) is also obtained in the course of these iterations. Each of these iterations is initialized by the solution of the calorically perfect shock wave equations (see reference *1*) using the local ratio of specific heats γ. Subroutines *Codelt* and *Cosigm* compute such calorically perfect initial estimates.

Subroutines *Todelt* and *Tosigm* only converge to reasonable answers if the equations are physically valid for the given upstream conditions and desired angles. Thus, the limiting static temperature and corresponding Mach number $M_{1,lim}$ must be determined prior to iterating for specific conditions; subroutine *sta2lim* (short for "station 2 limits") determines these limiting conditions. For a given σ, the limiting conditions are found at the Mach angle, where the shock strength and δ reduce to zero. For a given δ, a two-dimensional iteration procedure determines the conditions at which the weak and strong shock wave solutions are identical, that is, the Mach number at which $\delta_{max}(M)=\delta$. The δ_{max} for a given Mach number is determined in subroutine *parabt* by assuming a parabolic form of δ as a function of σ for a given T_1. The quadratic coefficients of the parabola are adjusted until a good fit of the curve apex is found, and the resulting quadratic equation is solved analytically for the extremum.

Postprocessor Subroutine

The *postout* subroutine in **postout.f** simply opens the **TPGpost.dat** file, writes the tabular data in Tecplot ASCII format, and closes the file upon completion. The FORTRAN *open* statement specifies a status of "*unknown*" to allow the file to be re-opened for additional output.

Other Subroutines

Many of the subroutines in Version 3.1 of the TPG code are unchanged since the publication of reference *2*. Specifically, these routines include those which evaluate c_p, the integral of c_p, and the integral of c_p/T, and are found in files **ntgrat.f** and **cpsubs.f**. The *trangej* subroutine, which finds appropriate temperature ranges and the corresponding polynomial curve fit for a given T, is also unchanged; it also records instances in which the curve fit temperature limits are exceeded and writes warning messages to output files. Finally, the *initd* and *Block Data* routines are basically unchanged from reference *2*, except that a few isolated variables have been added or deleted as the code has evolved. See reference *2* for additional details regarding any of these routines.

Database Files

The thermochemical data required by the TPG code for a given mixture of gases is defined in a database file to be read at execution time. A database for the standard composition of air is contained within the code and may be accessed as the default. However, for mixtures of other gases, or for more complete models of air, a separate database file may be provided. The format is simple and modular, grouped by species with a two-line header, and additional databases are easily constructed. A sample two-species database is shown in Table 4, and the format is described in some detail in references *2* and *3*.

Sample Tabular Output

Table 5 shows a sample of the tabular output in the single table format for a shock angle of 30° in air at T_t=400 K. Following the header information, described previously, are columns of data for the isentropic flow properties and the properties across the oblique shock wave. The column headings, in order from left to right, refer to the isentropic flow properties of Mach number M_1 (upstream of any shock wave), static temperature T_1, ratio of specific heats γ, static-to-total pressure ratio p_1/p_t, static-to-total density ratio ρ_1/ρ_t, static-to-total temperature ratio T_1/T_t, dynamic-to-total pressure ratio q/p_t, area ratio for expansion from sonic flow A/A^*, and local velocity divided by the sonic speed-of-sound V/a^*. The oblique shock properties continue as shock wave angle σ, flow deflection angle δ, Mach number downstream of the shock wave M_2, static pressure ratio across the shock p_2/p_1, density ratio across the shock ρ_2/ρ_1, static temperature ratio across the shock T_2/T_1, and the ratio of total pressures across the shock $p_{t,2}/p_{t,1}$. For a given shock angle, the minimum flow deflection is 0°, corresponding to a shock wave of zero strength, i.e., a Mach wave. Thus, the minimum Mach number of 2.0 for a 30° shock is determined by the equation for the Mach angle, equation (24). For all non-subsonic Mach numbers the code outputs an informative message stating the minimum σ(=μ) for that Mach number. At subsonic Mach numbers there is obviously no solution to the shock relations, as noted in the output. These informative messages do not appear in the two-table format; the shock wave table simply begins with the minimum Mach number $M_{1,lim}$ for which a solution exists.

Tables 6(a) and (b) illustrate the TPG tabular output for a constant flow deflection angle δ. Table 6(a) gives the weak shock solutions, and 6(b) gives the strong shock solutions (i.e., σ approaches 90° and M_2<1). The column headings and the subsonic notations are as in table 5. However, in this case the limiting Mach number is determined by the maximum flow deflection angle for which the flow would remain attached to the leading edge of a wedge with half-angle δ. That is, solutions to equations (10) and (15) only exist below some δ_{max}; solutions to equations (10) and (15) are double valued below δ_{max}. At Mach numbers below the corresponding limiting $M_{1,lim}$, an informative message notes the δ_{max}: zero at sonic conditions and increasing with M_1 to the specified δ. Note that the tables *always* include entries at stagnation, sonic, and limiting shock wave $M_{1,lim}$ conditions, even if these are not requested by the user.

Table 7 illustrates the ability of the TPG code to calculate flow properties across a sequence of shock waves, where each successive shock wave is dependent upon the flow conditions from the preceding one. The simple example consists of Mach 7 free stream flow being compressed by two 5° turns. The values of M_2 in the first set of oblique shock wave flow properties following the header become the values of M_1 in the second set. Version 3.1 treats the shock waves independently and generates unique table(s) for each. The resultant static pressure rise across the two shocks can be obtained by multiplying the individual pressure ratios. For example, at M_1=7.0: p_2/p_1=2.235, and M_2=6.104. At M_1=6.104: p_2/p_1=2.034, and M_2=5.398. The resultant static pressure rise is therefore 2.235 x 2.034 = 4.546. The other properties of density, temperature, and total pressure ratios across both shock waves are calculated in a similar fashion. A future version of TPG may condense the data into a single table and provide cumulative ratios automatically.

Oblique Shock Code Validation

The general polynomial curve fit methodology of the TPG code for thermally perfect properties was previously validated in references *2* and *3*. The oblique shock wave capabilities within the TPG code were validated in the same manner as were the basic isentropic flow and normal shock wave methods in these references, both in the calorically perfect and in the thermally perfect temperature regimes. In the current development, a normal shock wave is simply a special case of an oblique shock wave with σ=90°; the previous validations still hold for this special case.

Calorically Perfect Temperature Regime

The first validation test of the TPG code's oblique shock wave capability was the verification of accuracy in the temperature regime usually considered to be calorically perfect, with air as the test gas. In this temperature regime, the specific heat of air is nearly constant and therefore the TPG code results should be nearly identical to results obtained from the calorically perfect formulas of NACA Rep. 1135. For these test cases, the default data file for standard four-species air was used along with the default (standard) values for the mass fraction composition of air. The code default total temperature of 400 K was selected, a temperature considered within the calorically perfect temperature regime for air. The lower Mach number limit was defaulted to stagnation conditions and the upper Mach number limit was set to 10, with a Mach number increment of 0.1. In the case of real air at T_t=400 K, liquefaction would occur well before Mach 10; the data is presented to that extreme herein merely for comparison with the calorically perfect gas tables of NACA Rep. 1135 (which, incidentally, extend up to Mach 100). (All cases presented herein were run with the TPG code in the Mach number increment mode. See reference *2* for examples of the temperature increment mode.)

Figures 3(a-c) and 4(a-c) compare TPG calculations of M_2, δ, ρ_2/ρ_1, T_2/T_1, p_2/p_1, and $p_{t,2}/p_{t,1}$ for air with calorically perfect (γ=1.40) solutions at shock wave angles of 30° and 50°, respectively. Each variable is plotted versus upstream Mach number M_1. The differences are negligible as shown. Figures 5 and 6 show the same data presented as ratios of the thermally perfect values to the calorically perfect values. At σ=30°, the differences are less than 0.23% for all variables except total pressure ratio $p_{t,2}/p_{t,1}$. Similarly, for σ=50° the differences are less than 0.25%, except for total pressure ratio. Even for this most sensitive variable, the differences are less than 1%, and that value is approached only at the largest shock angle and for Mach numbers approaching 10. As noted in reference *2* for normal shock waves, these small differences actually represent the small amount of error associated with the calorically perfect gas assumption. A slight variation with temperature actually exists in the heat capacities even at such a low T_t, and is the cause of the variations seen in figures 5 and 6.

Thermally Perfect Temperature Regime

The properties for arbitrary oblique shock waves were verified for test cases involving standard four-species air at total temperatures of 1500 K and 3000 K, and at shock wave angles of 30° and 50°. Comparisons were made with results obtained via the imperfect gas relations of NACA Rep. 1135 (i.e, the Θ-equations for a diatomic gas) and with selected results from the calorically perfect gas assumption. The properties of δ, M_2, p_2/p_1, T_2/T_1, ρ_2/ρ_1, and $p_{t,2}/p_{t,1}$ are plotted versus the upstream Mach number M_1 in figures 7 and 8. Figures 7(a)-(f) show results for T_t=1500 K, a temperature well above the limits of the calorically perfect assumption for air, and figures 8(a)-(f) are for T_t=3000 K, an even more extreme case. The two thermally perfect gas methods agree extremely well. Cursory examination of the plots shows that imperfect gas effects increase with both total temperature and shock angle. For some flow conditions the differences appear to be negligible, but, for other conditions, the differences can be large. Also, not all properties appear to be equally sensitive to caloric imperfections.

The calculation for a total temperature of 3000 K is presented as an extreme case to illustrate application of the TPG code over an extended temperature range under the assumption of chemically frozen flow, i.e., fixed composition. The presentation is in the same spirit as that of references *5* and *6*, where data is presented to 5000 K and 6000 K, respectively. As always, users must keep in mind the applicability of the assumption of chemically frozen flow to a particular problem.

A more descriptive mode for examining the differences between the thermally perfect gas calculations and calorically perfect results is shown in figures 9(a)-(f). In these plots, the thermally perfect properties (δ, M_2, p_2/p_1, T_2/T_1, ρ_2/ρ_1, and $p_{t,2}/p_{t,1}$) are divided by the calorically perfect properties at identical values of M_1 to yield a measure of the imperfect gas effects. Results are shown for both total temperatures and both shock angles, for both the TPG code and the Θ-equation method of NACA Rep. 1135 (ref. *1*). In this format differences due to caloric imperfections are observed of 10% or greater for temperature ratio, density ratio, and total pressure ratio at the higher total temperature and greatest shock angle. Caloric imperfection differences on the order of 4-5% are observed for all variables except static pressure ratio, even at the lower total temperature. Also, the magnitudes of the caloric imperfections do not all vary uniformly with Mach number M_1. The effects on δ are largest at lower M_1, but are larger for other variables at higher M_1. For static pressure ratio the sign of the caloric imperfection effect changes as M_1 increases. Thus, the use of the calorically perfect relationships could result in substantial errors, particularly in the design or analysis of flows with a sequence of such shock waves. Finally, these results are shown assuming that M_1 is the control variable, i.e., the variable held fixed for both calorically and thermally perfect calculations. For other applications, the control variable might be the flow deflection angle δ, for example, and the magnitude of the caloric imperfection could be even greater. (Comparisons relative to the total, state 0, conditions, rather than state 1, would also yield larger effects of caloric imperfection.)

The differences between the two thermally perfect gas methods can be seen to be small (typically less than 0.25%). This excellent agreement verifies the accuracy of the TPG code with the derived thermally perfect gas relations for oblique shock waves based upon polynomial expressions for c_p. Although these test cases were all for air, which is a primarily diatomic gas, the TPG code is also valid for polyatomic gases. The utilization of a polynomial curve fit for c_p makes the TPG code applicable to any molecular structure of the gas, not just the diatomic structure upon which the Θ-equations are based.

Comparisons with CFD

As an additional validation of the TPG code's oblique shock wave capability, results were compared to computational fluid dynamics Euler solutions (i.e., inviscid flows). The CFD solutions were obtained using the General Aerodynamic Simulation Program (GASP), ref. *11*, of AeroSoft, Inc. GASP solves the integral form of the governing equations, including the full time-dependent Reynolds-averaged Navier-Stokes equations and various subsets: the Thin-Layer Navier-Stokes equations, the Parabolized Navier-Stokes equations, and the Euler equations. A generalized chemistry model and both equilibrium and non-equilibrium thermodynamics models are included. The discretized equations may be solved by space marching or by global iteration. The current computations utilized space marching (i.e., totally supersonic flow) for the inviscid Euler equations. Third-order upwind inviscid fluxes were calculated using Roe's split flux normal to the flow direction with Min-Mod flux limiting. The NASA Lewis Research Center equilibrium curve fits for specific heat (references *7*, *8* and *9*), of the same form employed within TPG, defined the thermodynamic characteristics of the gases. A 2-D grid of 20 uniformly-spaced computational cells per unit length was defined on a nondimensional domain (10 units long) above a simple wedge. The domain height was chosen so that the resulting oblique shock wave would pass through the downstream boundary (5 and 8.4 units for the two test cases, respectively).

The first CFD test case involved conditions representative of a generic high-speed inlet: thermally perfect air at M_1=4.8, T_1=1670 K and p_1=101325 N/m^2 (1 atmosphere) flowing over a 10° wedge. Figure 10 shows contours of pressure ratio p/p_1 for the GASP Euler solution with the shock wave computed by the TPG code (σ=19.415°) overlaid as a thick dashed line. The magnified view (see the inset) shows that the agreement in shock position is excellent, considering that GASP captures the shock over a number of cells and the TPG solution is a precise point-solution, that is, the shock wave is a true discontinuity. More detailed comparisons of M, p/p_1, T/T_1, and ρ/ρ_1 are shown in the line plots of figure 11(a)-(d). The data points shown were interpolated from the GASP solution field (e.g., figure 10) along a horizontal line at z=2.6 units above the wedge leading edge. The TPG solution is shown as a discontinuous solid line with the shock position calculated geometrically at that same lateral location of 2.6 units. Again, the agreement is excellent outside the region of shock capturing.

The Θ-equations of NACA Rep. 1135 are valid only for a single-species diatomic gas. Therefore, a second comparison with GASP was computed at arbitrary conditions designed to highlight the flexibility of the TPG code. The gas chosen was a two-species mixture of 20% steam and 80% CO_2 by mass, neither species being diatomic. Upstream conditions were set at

M_1=3.5, T_1=1200 K and p_1=101325 N/m^2. A rather severe wedge angle of 25° was selected and the 2-D GASP grid was constructed as before: 20 uniformly-spaced computational cells per unit length defined on a nondimensional domain (10 by 8.4 units to contain the expected shock wave). GASP required 282.4 cpu seconds to compute the solution on a Cray[2] Y-MP computer, not including grid generation and GASP input setup time (about 2 days). The TPG solution was practically instantaneous, computed on a Sun[3] Sparcstation 20 workstation. The resulting solutions are shown in figure 12, again with the TPG solution (σ=37.3037°) overlaid as a thick dashed line on the GASP pressure ratio contours. The magnified view in the inset again confirms the excellent agreement of the shock positions. The line plots of M, p/p_1, T/T_1, and ρ/ρ_1 shown in figure 13(a)-(d) confirm the accuracy of the TPG code for arbitrary mixtures of polyatomic gases. Since the TPG result is a precise point-solution, the overshoots seen in figure 13, and common to shock-capturing CFD codes, are eliminated. Similar to figure 11(a)-(d), the data points were interpolated from the GASP solution (figure 12) along a horizontal line at z=5.0 units above the wedge leading edge, and the TPG solution is shown as a discontinuous solid line with the shock position calculated at the same lateral location of 5 units.

Temperature Limits of the TPG Code

The TPG code provides valid results as long as its application is within the thermally perfect temperature regime for the gas of interest. If the code is used outside of the region for which c_p is a function of temperature only, then the thermally perfect results produced by this code will no longer accurately reflect what actually happens in nature. Dissociation will occur above some upper temperature limit, and will cause a deviation from thermally perfect theory. At the opposite extreme, below some lower temperature real gas effects will become important (i.e., intermolecular forces will not be negligible). The TPG code user must remain aware of these high and low temperature boundaries associated with the thermally perfect assumption for the particular gas(es) under consideration. Note that these are boundaries associated with the physical properties of the gas(es), and are distinct from the upper and lower temperature limits associated with the polynomial curve fits utilized within the TPG code. These latter curve fit limits are tracked within the code, and users are warned by the TPG code when these limits are exceeded. The limits of the thermally perfect assumption are the user's responsibility, and are dependent upon the specific gas properties and flow conditions. See reference *2* for a more detailed discussion of these temperature limits.

2. Cray Research, Inc., Minneapolis, MN 55402.
3. Sun Microsystems, Inc., Mountain View, CA 94043.

Conclusions

A set of compressible flow relations describing flow properties across oblique shock waves has been derived for a thermally perfect, calorically imperfect gas, and applied within the existing thermally perfect gas (TPG) computer code. The relations are based upon a value of c_p expressed as a polynomial function of temperature. The code now produces tables of compressible flow properties of oblique shock waves, as well as the properties of normal shock waves and basic isentropic flow from the original code, in a format similar to the tables for normal shock waves found in NACA Rep. 1135. The code results were validated in both the calorically perfect and the calorically imperfect, thermally perfect temperature regimes through comparisons with the theoretical methods of NACA Rep. 1135, and with a state-of-the-art computational fluid dynamics code. The TPG code is applicable to any type of gas or mixture of gases and is not restricted to only diatomic gases as are the thermally perfect methods of NACA Rep. 1135.

The TPG code computes properties of oblique shock waves for given shock wave angles, or for given flow deflection (wedge) angles, including both strong and weak shock waves. Normal shock waves are a special case of an oblique shock wave. The code also allows calculation of a sequence of shocks where each successive shock wave is dependent upon the flow conditions from the preceding one. Both tabular output and output for plotting and post-processing are available. Typical computation time is on the order of 1-5 seconds for most computer workstations or personal computers. The user effort required is minimal, and consists of only simple answers to 14 interactive questions (or less) per table generated. Thermally perfect properties of flows through oblique shock waves may be computed with less effort than has traditionally been expended to compute calorically perfect properties. Errors incurred from using calorically perfect gas relations, instead of the thermally perfect gas equations, in the thermally perfect temperature regime have been shown to approach 10% for some applications.

The TPG code is available from the NASA Langley Software Server (LSS) on the World-Wide-Web at the following address:

http://www.larc.nasa.gov/LSS

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Appendix A

Equations for Numerical Implementation

Equations (7) and (14) may be written as

$$F_1(\sigma, \delta, T_2) = \frac{\tan(\sigma-\delta)}{\tan\sigma} - \frac{u_2}{u_1} = 0 \quad \text{(A1)}$$

and

$$F_2(\sigma, \delta, T_2) = \frac{RT_1}{u_1} + u_1 - \frac{RT_2}{u_2} - u_2 = 0 \quad \text{(A2)}$$

where state 1 conditions T_1 and u_1 are assumed to be known, and u_2 is a function of σ, δ, and T_2, as seen from equations (9) and (16), reproduced here for completeness.

$$u_2 = V_2 \sin(\sigma-\delta) \quad \text{(A3)}$$

$$V_2^2 = 2\int_{T_2}^{T_t} c_p dT \quad \text{(A4)}$$

Thus, there are two nonlinear equations for three unknowns. Typically, either σ or δ is known, and the equations may be solved numerically for the remaining angle and T_2 by Newton iteration.

In the case of the shock wave angle σ being given, the equations may be rewritten as

$$F_i(\sigma, \delta, T_2) = G_i(\delta, T_2)\big|_\sigma\,, \text{ for } i=1,2. \quad \text{(A5)}$$

That is,

$$G_1(\delta, T_2) = \frac{\tan(\sigma-\delta)}{\tan\sigma} - \frac{u_2}{u_1} = 0 \quad \text{(A6)}$$

and

$$G_2(\delta, T_2) = \frac{RT_1}{u_1} + u_1 - \frac{RT_2}{u_2} - u_2 = 0 \quad \text{(A7)}$$

Now u_2 can also be written as

$$u_2^2 = V_2^2 - w^2 = 2\int_{T_2}^{T_t} c_p dT - w^2 \quad \text{(A8)}$$

Therefore, u_2 is a function of only T_2 if σ is given, and equation (A7) is actually

$$G_2(\delta, T_2) = G_2(T_2) = 0 \quad \text{(A9)}$$

Once equation (A9) is solved for T_2, V_2 is known from equation (A4), u_2 from equation (A3), and δ may be found from equation (A6) or simply from

$$\cos(\sigma-\delta) = \frac{w}{V_2} \quad \text{(A10)}$$

In the case of the flow deflection angle δ being given, equations (A1) and (A2) are a system of two nonlinear equations for the two unknowns σ and T_2, and may be written as

$$F_1(\sigma, T_2) = \frac{\tan(\sigma-\delta)}{\tan\sigma} - \frac{V_2\sin(\sigma-\delta)}{V_1\sin\sigma} = 0 \quad \text{(A11)}$$

and

$$F_2(\sigma, T_2) = \frac{RT_1}{V_1\sin\sigma} + V_1\sin\sigma - \frac{RT_2}{V_2\sin(\sigma-\delta)} - V_2\sin(\sigma-\delta) \quad \text{(A12)}$$

The solution can be found by application of Newton's method to a system of equations, similar to the application to equation (A9).

For equation (A9), a single equation of a single unknown, Newton's iterative method can be written

$$\left(\frac{dG_2}{dT_2}\right)^k (\Delta T_2)^{k+1} + G_2^k = 0 \quad \text{(A13)}$$

where the superscripts denote the iteration step. That is, the function G_2 and the derivative of G_2 are evaluated using values at the current, or *k'th*, iterative approximation step in order to solve for the *k+1'th* correction to the approximate solution. The differential equation is then replaced by the following algebraic equation

$$(\Delta T_2)^{k+1} = T_2^{k+1} - T_2^k = G_2^k \bullet \left[\left(\frac{dG_2}{dT_2}\right)^k\right]^{-1} \quad \text{(A14)}$$

For a system of equations, the functional evaluation $G_2{}^k$ becomes a vector, and the derivative becomes a matrix of partial derivatives which must be inverted. The correction term

ΔT_2 becomes a vector of the unknowns σ and T_2, in the case of equations (A11) and (A12). Equation (A14) is thus replaced by a system of two algebraic equations for the two unknowns.

Newton's method requires an initial estimate of the solution. Within the TPG code, the initial approximation is given by the solution of the oblique shock wave relations for a calorically perfect gas at the local conditions (i.e., M_1, and γ_1). NACA Rep. 1135 summarizes these equations, as do many compressible flow textbooks.

Newton's method applied to equations (A9) and (A11-12) does not converge for $M_1 < M_{1,lim}$ where oblique shock waves cannot exist, as discussed previously in the section on *Oblique Shock Relations*. For the case of known σ, the limiting M_1 is defined by equation (24), where $\mu = \sigma$. For the case of known δ, the limiting M_1 is defined along the curve labeled δ_{max} in figure 2. Within the TPG code, an additional nonlinear iteration searches for the point on the curve at which $\delta_{max} = \delta$. At each step of the search, the value of δ_{max} for a given M_1 is found by parabolic approximation of the curve apex.

Table 3: Sample TPG.out header information

```
 ________________________________________
|    Thermally Perfect Gas Properties Code    |
|              TPG, Version 3.1.0             |
|                                             |
|        NASA  Langley Research Center        |
 ________________________________________

Table of Thermally Perfect Compressible Flow Properties
Gaseous Mixture:    Air: 4-Species Mixture of N2, O2, Argon, and CO2
Database file name:  [ Default database of Air Mixture ]
Species Names are:
                N2   ,        O2   ,        Argon,       CO2  ,
Species Mass Fractions are:
                0.75530      0.23140      0.01290      0.00040
Species Mole Fractions are:
                0.78092      0.20946      0.00935      0.00026
Mixture Properties:
                      Molecular Weight  =   28.9663
                           Gas Constant  =   2.87035E+02 J/(kg*K)
                 Polynomial Coefficients :   cp/R = Sum{A(i)*T^(i–2)}
                     80.0 < T <  1000.0 degrees K
       –3.7319821D+00      5.4196701D–01      3.4693586D+00      3.8353798D–04
       –2.7653130D–06      8.1886142D–09     –7.7368690D–12      2.4348723D–15
                  1000.0 < T <  6000.0 degrees K
        2.3769851D+05     –1.2440527D+03      5.1266690D+00     –2.0400644D–04
        6.8321801D–08     –1.0553542D–11      6.6450071D–16      0.0000000D+00

Total Temperature =   400.000 K
```

Table 4: Sample thermochemical database file

```
# of species      #of Temperature ranges : NASP TM 1107 + Mods.
  2                 2
Name:             Molecular Wt.
N2                28.0160
tmin              tmax
 20.              1000.
Cp/R Coefficients: c1(–2) —> c1(5)
 –1.33984200E+01      1.34280300E+00     3.45742000e+00      5.74727600E–04
 –3.21711900E–06      7.50775400E–09    –5.90150500E–12      1.50979900E–15
tmin              tmax
1000.             6000.
Cp/R Coefficients: c2(–2) —> c2(5)
   5.87702841E+05    –2.23921563E+03     6.06686971E+00    –6.13957913E–04
   1.49178026E–07    –1.92307130E–11     1.06193594E–15      0.00000000E+00
Name:             Molecular Wt.
O2                32.0000
tmin              tmax
 30.              1000.
Cp/R Coefficients: c1(–2) —> c1(5)
   3.88517500E+01    –2.70630800E+00     3.56119600E+00    –3.32782400E–04
 –1.18148000E–06      1.10853500E–08    –1.49299400E–11      5.99553800E–15
tmin              tmax
1000.             6000.
Cp/R Coefficients: c2(–2) —> c2(5)
 –1.05642070E+06      2.41123849E+03     1.73474238E+00      1.31512292E–03
 –2.29995151E–07      2.13144378E–11    –7.87498771E–16      0.00000000E+00
```

Table 5: Sample TPG tabular output for constant shock wave angle

```
------------------------------------------
| Thermally Perfect Gas Properties Code |
|          TPG, Version 3.1.0            |
|                                        |
|     NASA  Langley Research Center      |
------------------------------------------

Table of Thermally Perfect Compressible Flow Properties
Gaseous Mixture:   Air: 4-Species Mixture of N2, O2, Argon, and CO2
Database file name: [ Default database of Air Mixture ]
Species Names are:
               N2   ,    O2   ,    Argon,    CO2  ,
Species Mass Fractions are:
             0.75530   0.23140   0.01290   0.00040
Species Mole Fractions are:
             0.78092   0.20946   0.00935   0.00026
Mixture Properties:
                 Molecular Weight =  28.9663
                     Gas Constant = 2.87035E+02 J/(kg*K)
          Polynomial Coefficients : cp/R = Sum{A(i)*T^(i-2)}
             80.0 < T <  1000.0 degrees K
     -3.7319821D+00   5.4196701D-01   3.4693586D+00   3.8353798D-04
     -2.7653130D-06   8.1886142D-09  -7.7368690D-12   2.4348723D-15
           1000.0 < T <  6000.0 degrees K
      2.3769851D+05  -1.2440527D+03   5.1266690D+00  -2.0400644D-04
      6.8321801D-08  -1.0553542D-11   6.6450071D-16   0.0000000D+00

Total Temperature =   400.000 K
```

ISENTROPIC FLOW PROPERTIES ---> OBLIQUE SHOCK WAVE FLOW PROPERTIES (2=downstream, 1=upstream) --->

M	T(K)	Gamma	P/Pt	RHO/RHOt	T/Tt	q/Pt	A/A*	V/a*	ShokAngl	FloDflec	M2	P2/P1	RHO2/RHO1	T2/T1	Pt2/Pt1
0.000	400.0	1.3949	1.000E+00	1.000E+00	1.0000	0.000E+00	infinite	0.00000	**	Subsonic: Not Applicable --->					
0.200	396.9	1.3951	9.726E-01	9.803E-01	0.9922	2.714E-02	2.966E+00	0.21784	**	Subsonic: Not Applicable --->					
0.400	387.7	1.3956	8.959E-01	9.242E-01	0.9693	1.000E-01	1.591E+00	0.43073	**	Subsonic: Not Applicable --->					
0.600	373.4	1.3965	7.844E-01	8.403E-01	0.9335	1.972E-01	1.189E+00	0.63422	**	Subsonic: Not Applicable --->					
0.800	355.0	1.3975	6.564E-01	7.397E-01	0.8874	2.935E-01	1.038E+00	0.82478	**	Subsonic: Not Applicable --->					
1.000	333.7	1.3985	5.285E-01	6.335E-01	0.8343	3.695E-01	1.000E+00	1.00000	**	Minimum Oblique Shock Wave Angle = 90.000					
1.200	310.9	1.3994	4.124E-01	5.305E-01	0.7773	4.155E-01	1.031E+00	1.15866	**	Minimum Oblique Shock Wave Angle = 56.443					
1.400	287.7	1.4001	3.141E-01	4.368E-01	0.7192	4.310E-01	1.115E+00	1.30057	**	Minimum Oblique Shock Wave Angle = 45.585					
1.600	264.8	1.4006	2.351E-01	3.551E-01	0.6620	4.214E-01	1.251E+00	1.42631	**	Minimum Oblique Shock Wave Angle = 38.682					
1.800	242.9	1.4010	1.739E-01	2.863E-01	0.6072	3.946E-01	1.440E+00	1.53700	**	Minimum Oblique Shock Wave Angle = 33.749					
2.000	222.3	1.4012	1.277E-01	2.297E-01	0.5558	3.577E-01	1.688E+00	1.63404	30.0000	0.0000	2.000	1.000E+00	1.000E+00	1.000E+00	1.000E+00
2.200	203.3	1.4013	9.341E-02	1.838E-01	0.5083	3.168E-01	2.005E+00	1.71892	30.0000	3.7160	2.059	1.245E+00	1.169E+00	1.065E+00	9.989E-01
2.400	185.9	1.4013	6.833E-02	1.470E-01	0.4648	2.758E-01	2.403E+00	1.79311	30.0000	6.7123	2.130	1.514E+00	1.341E+00	1.128E+00	9.928E-01
2.600	170.1	1.4013	5.008E-02	1.178E-01	0.4252	2.372E-01	2.895E+00	1.85799	30.0000	9.1421	2.208	1.805E+00	1.515E+00	1.191E+00	9.794E-01
2.800	155.8	1.4013	3.684E-02	9.460E-02	0.3894	2.023E-01	3.497E+00	1.91480	30.0000	11.1281	2.287	2.120E+00	1.689E+00	1.255E+00	9.582E-01
3.000	142.8	1.4013	2.722E-02	7.624E-02	0.3571	1.717E-01	4.229E+00	1.96463	30.0000	12.7656	2.367	2.459E+00	1.861E+00	1.321E+00	9.298E-01
3.200	131.2	1.4012	2.024E-02	6.169E-02	0.3280	1.452E-01	5.112E+00	2.00845	30.0000	14.1280	2.444	2.821E+00	2.031E+00	1.389E+00	8.953E-01
3.400	120.7	1.4012	1.514E-02	5.015E-02	0.3018	1.226E-01	6.171E+00	2.04707	30.0000	15.2714	2.520	3.206E+00	2.196E+00	1.460E+00	8.558E-01
3.600	111.3	1.4012	1.140E-02	4.096E-02	0.2783	1.035E-01	7.431E+00	2.08122	30.0000	16.2391	2.592	3.614E+00	2.357E+00	1.533E+00	8.128E-01
3.800	102.8	1.4012	8.643E-03	3.362E-02	0.2571	8.743E-02	8.924E+00	2.11149	30.0000	17.0643	2.661	4.046E+00	2.514E+00	1.610E+00	7.676E-01
4.000	95.2	1.4012	6.599E-03	2.773E-02	0.2380	7.397E-02	1.068E+01	2.13842	30.0000	17.7733	2.727	4.501E+00	2.664E+00	1.689E+00	7.211E-01

Table 6: Sample TPG tabular outputs for constant flow deflection angle

(a) Weak shock wave solutions

```
 -----------------------------------------
 | Thermally Perfect Gas Properties Code |
 |           TPG, Version 3.1.0          |
 |                                       |
 |     NASA  Langley Research Center     |
 -----------------------------------------

 Table of Thermally Perfect Compressible Flow Properties
 Gaseous Mixture:   Air: 4-Species Mixture of N2, O2, Argon, and CO2
 Database file name: [ Default database of Air Mixture ]
 Species Names are:
                N2   ,    O2   ,    Argon,    CO2  ,
 Species Mass Fractions are:
            0.75530   0.23140   0.01290   0.00040
 Species Mole Fractions are:
            0.78092   0.20946   0.00935   0.00026
 Mixture Properties:
                 Molecular Weight =  28.9663
                     Gas Constant = 2.87035E+02 J/(kg*K)
          Polynomial Coefficients : cp/R = Sum{A(i)*T^(i-2)}
            80.0 < T <  1000.0 degrees K
      -3.7319821D+00   5.4196701D-01   3.4693586D+00   3.8353798D-04
      -2.7653130D-06   8.1886142D-09  -7.7368690D-12   2.4348723D-15
          1000.0 < T <  6000.0 degrees K
       2.3769851D+05  -1.2440527D+03   5.1266690D+00  -2.0400644D-04
       6.8321801D-08  -1.0553542D-11   6.6450071D-16   0.0000000D+00

 Total Temperature =   400.000 K
```

ISENTROPIC FLOW PROPERTIES ---> OBLIQUE SHOCK WAVE FLOW PROPERTIES (2=downstream, 1=upstream) --->

M	T(K)	Gamma	P/Pt	RHO/RHOt	T/Tt	q/Pt	A/A*	V/a*	ShokAngl	FloDflec	M2	P2/P1	RHO2/RHO1	T2/T1	Pt2/Pt1
0.000	400.0	1.3949	1.000E+00	1.000E+00	1.0000	0.000E+00	infinite	0.00000	**	Subsonic: Not Applicable --->					
0.200	396.9	1.3951	9.726E-01	9.803E-01	0.9922	2.714E-02	2.966E+00	0.21784	**	Subsonic: Not Applicable --->					
0.400	387.7	1.3956	8.959E-01	9.242E-01	0.9693	1.000E-01	1.591E+00	0.43073	**	Subsonic: Not Applicable --->					
0.600	373.4	1.3965	7.844E-01	8.403E-01	0.9335	1.972E-01	1.189E+00	0.63422	**	Subsonic: Not Applicable --->					
0.800	355.0	1.3975	6.564E-01	7.397E-01	0.8874	2.935E-01	1.038E+00	0.82478	**	Subsonic: Not Applicable --->					
1.000	333.7	1.3985	5.285E-01	6.335E-01	0.8343	3.695E-01	1.000E+00	1.00000	**	Maximum Attached-flow Shock Deflection Angle = 0.000					
1.200	310.9	1.3994	4.124E-01	5.305E-01	0.7773	4.155E-01	1.031E+00	1.15866	**	Maximum Attached-flow Shock Deflection Angle = 3.953					
1.400	287.7	1.4001	3.141E-01	4.368E-01	0.7192	4.310E-01	1.115E+00	1.30057	**	Maximum Attached-flow Shock Deflection Angle = 9.444					
1.600	264.8	1.4006	2.351E-01	3.551E-01	0.6620	4.214E-01	1.251E+00	1.42631	**	Maximum Attached-flow Shock Deflection Angle = 14.671					
1.800	242.9	1.4010	1.739E-01	2.863E-01	0.6072	3.946E-01	1.440E+00	1.53700	**	Maximum Attached-flow Shock Deflection Angle = 19.201					
1.839	238.7	1.4010	1.637E-01	2.743E-01	0.5969	3.879E-01	1.483E+00	1.55704	64.9121	20.0000	0.920	3.073E+00	2.143E+00	1.434E+00	8.696E-01
2.000	222.3	1.4012	1.277E-01	2.297E-01	0.5558	3.577E-01	1.688E+00	1.63404	53.4172	20.0000	1.211	2.844E+00	2.042E+00	1.393E+00	8.929E-01
2.200	203.3	1.4013	9.341E-02	1.838E-01	0.5083	3.168E-01	2.005E+00	1.71892	47.9823	20.0000	1.403	2.951E+00	2.089E+00	1.413E+00	8.821E-01
2.400	185.9	1.4013	6.833E-02	1.470E-01	0.4648	2.758E-01	2.403E+00	1.79311	44.3478	20.0000	1.568	3.118E+00	2.160E+00	1.444E+00	8.650E-01
2.600	170.1	1.4013	5.008E-02	1.178E-01	0.4252	2.372E-01	2.895E+00	1.85799	41.6351	20.0000	1.719	3.316E+00	2.241E+00	1.479E+00	8.443E-01
2.800	155.8	1.4013	3.684E-02	9.460E-02	0.3894	2.023E-01	3.497E+00	1.91480	39.5046	20.0000	1.860	3.536E+00	2.328E+00	1.519E+00	8.211E-01
3.000	142.8	1.4013	2.722E-02	7.624E-02	0.3571	1.717E-01	4.229E+00	1.96463	37.7787	20.0000	1.993	3.775E+00	2.417E+00	1.562E+00	7.959E-01
3.200	131.2	1.4012	2.024E-02	6.169E-02	0.3280	1.452E-01	5.112E+00	2.00845	36.3501	20.0000	2.119	4.031E+00	2.509E+00	1.607E+00	7.691E-01
3.400	120.7	1.4012	1.514E-02	5.015E-02	0.3018	1.226E-01	6.171E+00	2.04707	35.1484	20.0000	2.239	4.304E+00	2.601E+00	1.655E+00	7.410E-01
3.600	111.3	1.4012	1.140E-02	4.096E-02	0.2783	1.035E-01	7.431E+00	2.08122	34.1245	20.0000	2.353	4.593E+00	2.693E+00	1.705E+00	7.120E-01
3.800	102.8	1.4012	8.643E-03	3.362E-02	0.2571	8.743E-02	8.924E+00	2.11149	33.2431	20.0000	2.462	4.897E+00	2.785E+00	1.758E+00	6.823E-01
4.000	95.2	1.4012	6.599E-03	2.773E-02	0.2380	7.397E-02	1.068E+01	2.13842	32.4776	20.0000	2.566	5.217E+00	2.876E+00	1.814E+00	6.523E-01

Table 6: Sample TPG tabular outputs for constant flow deflection angle

(b) Strong shock wave solutions

```
 -----------------------------------------
 | Thermally Perfect Gas Properties Code |
 |          TPG, Version 3.1.0           |
 |                                       |
 |     NASA  Langley Research Center     |
 -----------------------------------------

 Table of Thermally Perfect Compressible Flow Properties
 Gaseous Mixture:   Air: 4-Species Mixture of N2, O2, Argon, and CO2
 Database file name: [ Default database of Air Mixture ]
 Species Names are:
               N2   ,    O2   ,    Argon,    CO2  ,
 Species Mass Fractions are:
             0.75530   0.23140   0.01290   0.00040
 Species Mole Fractions are:
             0.78092   0.20946   0.00935   0.00026
 Mixture Properties:
                 Molecular Weight =  28.9663
                     Gas Constant = 2.87035E+02 J/(kg*K)
          Polynomial Coefficients : cp/R = Sum{A(i)*T^(i-2)}
             80.0 < T <  1000.0 degrees K
      -3.7319821D+00   5.4196701D-01   3.4693586D+00   3.8353798D-04
      -2.7653130D-06   8.1886142D-09  -7.7368690D-12   2.4348723D-15
           1000.0 < T <  6000.0 degrees K
       2.3769851D+05  -1.2440527D+03   5.1266690D+00  -2.0400644D-04
       6.8321801D-08  -1.0553542D-11   6.6450071D-16   0.0000000D+00

 Total Temperature =   400.000 K

ISENTROPIC FLOW PROPERTIES --->                                                      OBLIQUE SHOCK WAVE FLOW PROPERTIES   (2=downstream, 1=upstream) --->

  M     T(K)   Gamma    P/Pt     RHO/RHOt   T/Tt      q/Pt       A/A*       V/a*   ShokAngl  FloDflec    M2     P2/P1    RHO2/RHO1   T2/T1     Pt2/Pt1

0.000   400.0  1.3949  1.000E+00  1.000E+00  1.0000  0.000E+00  infinite   0.00000      **  Subsonic:  Not Applicable  --->
0.200   396.9  1.3951  9.726E-01  9.803E-01  0.9922  2.714E-02  2.966E+00  0.21784      **  Subsonic:  Not Applicable  --->
0.400   387.7  1.3956  8.959E-01  9.242E-01  0.9693  1.000E-01  1.591E+00  0.43073      **  Subsonic:  Not Applicable  --->
0.600   373.4  1.3965  7.844E-01  8.403E-01  0.9335  1.972E-01  1.189E+00  0.63422      **  Subsonic:  Not Applicable  --->
0.800   355.0  1.3975  6.564E-01  7.397E-01  0.8874  2.935E-01  1.038E+00  0.82478      **  Subsonic:  Not Applicable  --->
1.000   333.7  1.3985  5.285E-01  6.335E-01  0.8343  3.695E-01  1.000E+00  1.00000      **  Maximum Attached-flow Shock Deflection Angle =  0.000
1.200   310.9  1.3994  4.124E-01  5.305E-01  0.7773  4.155E-01  1.031E+00  1.15866      **  Maximum Attached-flow Shock Deflection Angle =  3.953
1.400   287.7  1.4001  3.141E-01  4.368E-01  0.7192  4.310E-01  1.115E+00  1.30057      **  Maximum Attached-flow Shock Deflection Angle =  9.444
1.600   264.8  1.4006  2.351E-01  3.551E-01  0.6620  4.214E-01  1.251E+00  1.42631      **  Maximum Attached-flow Shock Deflection Angle = 14.671
1.800   242.9  1.4010  1.739E-01  2.863E-01  0.6072  3.946E-01  1.440E+00  1.53700      **  Maximum Attached-flow Shock Deflection Angle = 19.201
1.839   238.7  1.4010  1.637E-01  2.743E-01  0.5969  3.879E-01  1.483E+00  1.55704   64.9121   20.0000   0.920  3.073E+00  2.143E+00  1.434E+00  8.696E-01
2.000   222.3  1.4012  1.277E-01  2.297E-01  0.5558  3.577E-01  1.688E+00  1.63404   74.3031   20.0000   0.728  4.163E+00  2.557E+00  1.628E+00  7.555E-01
2.200   203.3  1.4013  9.341E-02  1.838E-01  0.5083  3.168E-01  2.005E+00  1.71892   77.5677   20.0000   0.657  5.224E+00  2.882E+00  1.812E+00  6.517E-01
2.400   185.9  1.4013  6.833E-02  1.470E-01  0.4648  2.758E-01  2.403E+00  1.79311   79.4141   20.0000   0.613  6.333E+00  3.163E+00  2.002E+00  5.576E-01
2.600   170.1  1.4013  5.008E-02  1.178E-01  0.4252  2.372E-01  2.895E+00  1.85799   80.6332   20.0000   0.582  7.519E+00  3.411E+00  2.204E+00  4.735E-01
2.800   155.8  1.4013  3.684E-02  9.460E-02  0.3894  2.023E-01  3.497E+00  1.91480   81.5016   20.0000   0.559  8.789E+00  3.633E+00  2.419E+00  3.999E-01
3.000   142.8  1.4013  2.722E-02  7.624E-02  0.3571  1.717E-01  4.229E+00  1.96463   82.1502   20.0000   0.540  1.015E+01  3.832E+00  2.648E+00  3.367E-01
3.200   131.2  1.4012  2.024E-02  6.169E-02  0.3280  1.452E-01  5.112E+00  2.00845   82.6513   20.0000   0.525  1.159E+01  4.010E+00  2.891E+00  2.830E-01
3.400   120.7  1.4012  1.514E-02  5.015E-02  0.3018  1.226E-01  6.171E+00  2.04707   83.0484   20.0000   0.513  1.313E+01  4.170E+00  3.149E+00  2.377E-01
3.600   111.3  1.4012  1.140E-02  4.096E-02  0.2783  1.035E-01  7.431E+00  2.08122   83.3695   20.0000   0.502  1.476E+01  4.314E+00  3.423E+00  1.998E-01
3.800   102.8  1.4012  8.643E-03  3.362E-02  0.2571  8.743E-02  8.924E+00  2.11149   83.6336   20.0000   0.493  1.649E+01  4.443E+00  3.711E+00  1.682E-01
4.000    95.2  1.4012  6.599E-03  2.773E-02  0.2380  7.397E-02  1.068E+01  2.13842   83.8536   20.0000   0.486  1.830E+01  4.559E+00  4.015E+00  1.419E-01
```

Table 7: Sample TPG output for a sequence of shock waves

```
                   -----------------------------------------
                   | Thermally Perfect Gas Properties Code |
                   |          TPG, Version 3.1.0           |
                   |                                       |
                   |     NASA  Langley Research Center     |
                   -----------------------------------------

                   Table of Thermally Perfect Compressible Flow Properties
                   Gaseous Mixture:   Air: 4-Species Mixture of N2, O2, Argon, and CO2
                   Database file name: [ Default database of Air Mixture ]
                   Species Names are:
                                 N2   ,    O2   ,    Argon,    CO2  ,
                   Species Mass Fractions are:
                                0.75530   0.23140   0.01290   0.00040
                   Species Mole Fractions are:
                                0.78092   0.20946   0.00935   0.00026
                   Mixture Properties:
                                    Molecular Weight =  28.9663
                                        Gas Constant = 2.87035E+02 J/(kg*K)
                             Polynomial Coefficients : cp/R = Sum{A(i)*T^(i-2)}
                                80.0 < T <  1000.0 degrees K
                        -3.7319821D+00   5.4196701D-01   3.4693586D+00   3.8353798D-04
                        -2.7653130D-06   8.1886142D-09  -7.7368690D-12   2.4348723D-15
                              1000.0 < T <  6000.0 degrees K
                         2.3769851D+05  -1.2440527D+03   5.1266690D+00  -2.0400644D-04
                         6.8321801D-08  -1.0553542D-11   6.6450071D-16   0.0000000D+00

                   Total Temperature =  1500.000 K

ISENTROPIC FLOW PROPERTIES --->                                                       OBLIQUE SHOCK WAVE FLOW PROPERTIES   (2=downstream, 1=upstream) --->

  M     T(K)    Gamma     P/Pt     RHO/RHOt   T/Tt      q/Pt        A/A*       V/a*   ShokAngl  FloDflec    M2     P2/P1    RHO2/RHO1   T2/T1      Pt2/Pt1

0.000  1500.0  1.3107  1.000E+00  1.000E+00  1.0000  0.000E+00   infinite   0.00000      **  Subsonic:  Not Applicable  --->
1.000  1295.6  1.3187  5.422E-01  6.277E-01  0.8637  3.575E-01  1.000E+00   1.00000      **  Maximum Attached-flow Shock Deflection Angle =  0.000
1.231  1208.9  1.3230  4.077E-01  5.059E-01  0.8059  4.085E-01  1.042E+00   1.19069   71.1361    5.0000   0.945  1.408E+00  1.295E+00  1.088E+00  9.956E-01
7.000   150.8  1.4013  2.078E-04  2.068E-03  0.1005  7.135E-03  1.233E+02   2.46140   11.8273    5.0000   6.104  2.235E+00  1.749E+00  1.278E+00  9.491E-01

                   Total Temperature =  1500.000 K

ISENTROPIC FLOW PROPERTIES --->                                                       OBLIQUE SHOCK WAVE FLOW PROPERTIES   (2=downstream, 1=upstream) --->

  M     T(K)    Gamma     P/Pt     RHO/RHOt   T/Tt      q/Pt        A/A*       V/a*   ShokAngl  FloDflec    M2     P2/P1    RHO2/RHO1   T2/T1      Pt2/Pt1

0.000  1500.0  1.3107  1.000E+00  1.000E+00  1.0000  0.000E+00   infinite   0.00000      **  Subsonic:  Not Applicable  --->
0.945  1315.1  1.3179  5.768E-01  6.579E-01  0.8767  3.393E-01  1.003E+00   0.95158      **  Subsonic:  Not Applicable  --->
1.000  1295.6  1.3187  5.422E-01  6.277E-01  0.8637  3.575E-01  1.000E+00   1.00000      **  Maximum Attached-flow Shock Deflection Angle =  0.000
1.231  1208.9  1.3230  4.077E-01  5.059E-01  0.8059  4.085E-01  1.042E+00   1.19069   71.1361    5.0000   0.945  1.408E+00  1.295E+00  1.088E+00  9.956E-01
6.104   192.7  1.4013  4.895E-04  3.811E-03  0.1284  1.278E-02  6.789E+01   2.42635   13.0011    5.0000   5.398  2.034E+00  1.643E+00  1.238E+00  9.646E-01
```

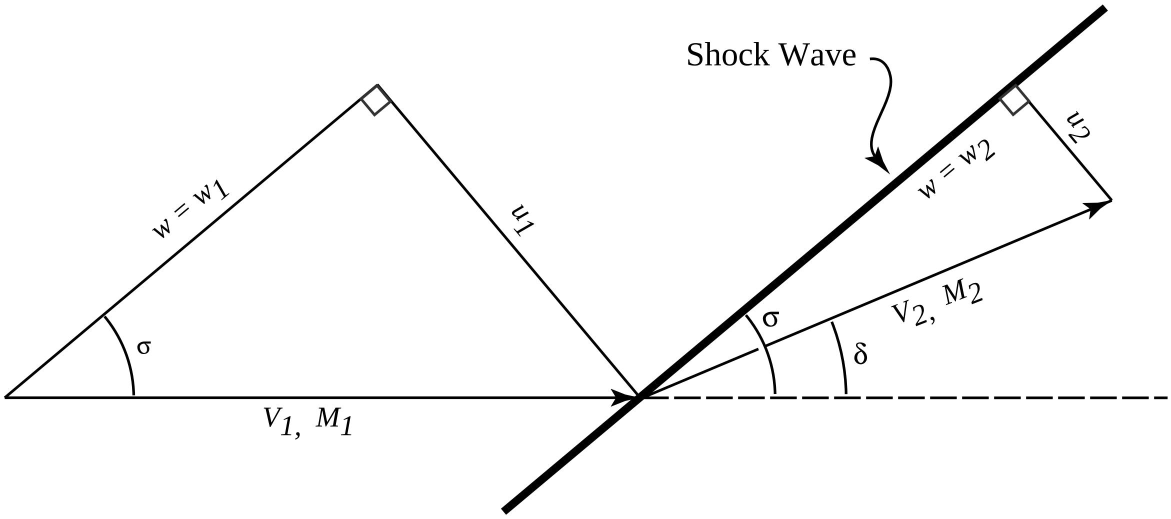


Figure 1. Geometric relationships of oblique shock waves.

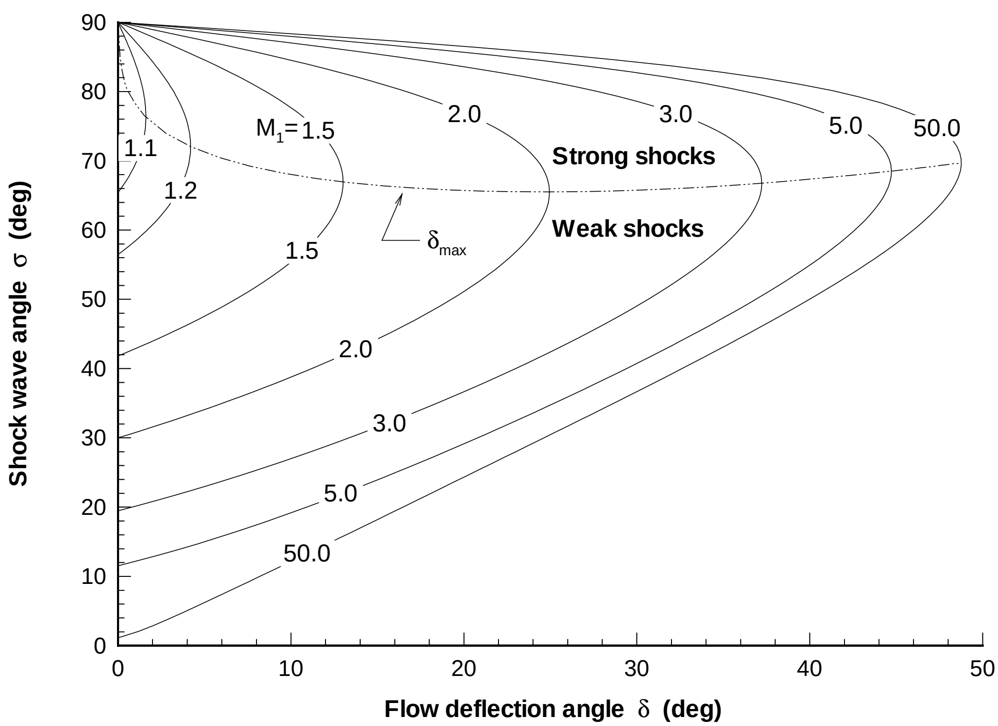
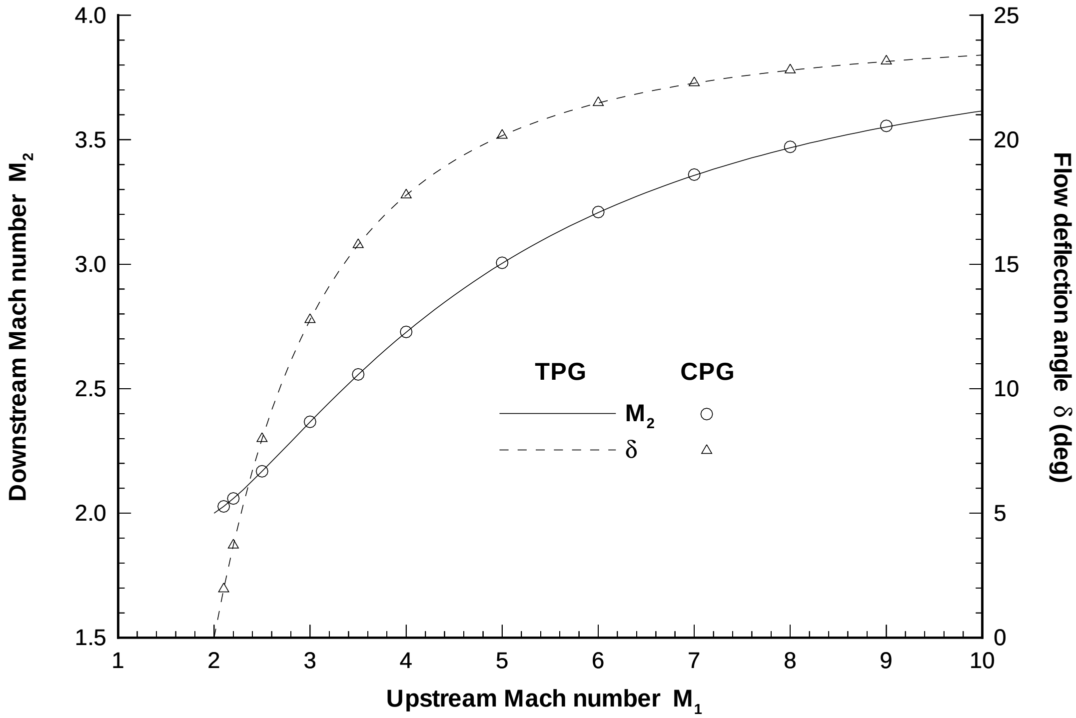
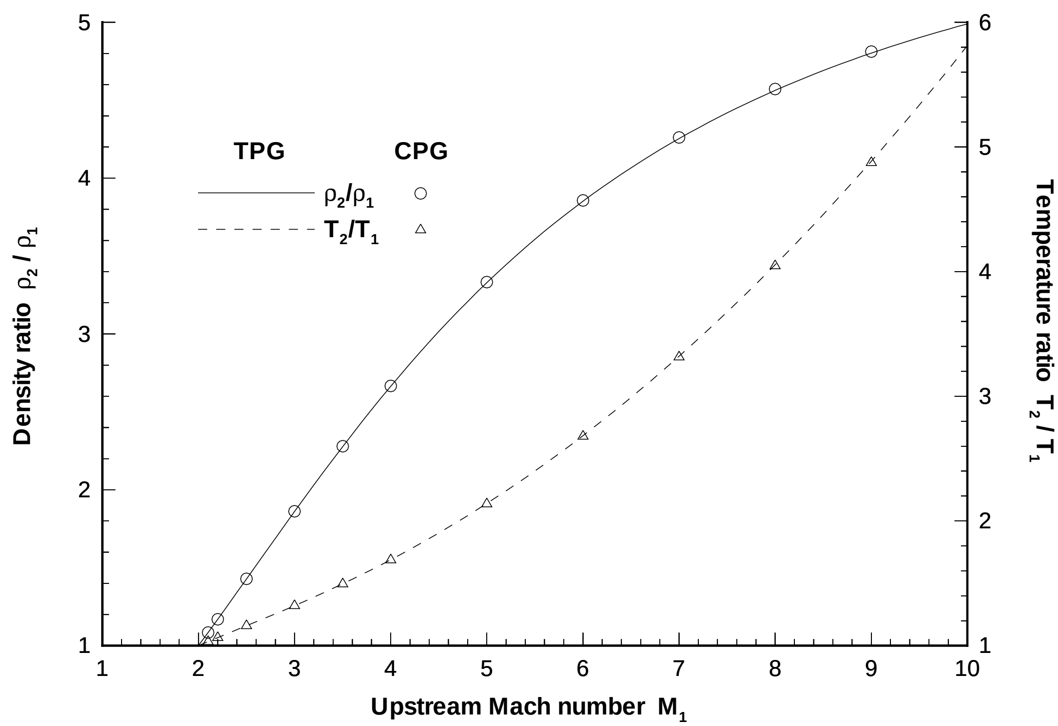


Figure 2. Contours of upstream Mach number M_1 for given shock wave angle σ and flow deflection angle δ: thermally perfect air at an arbitrary T_t=3000 K.

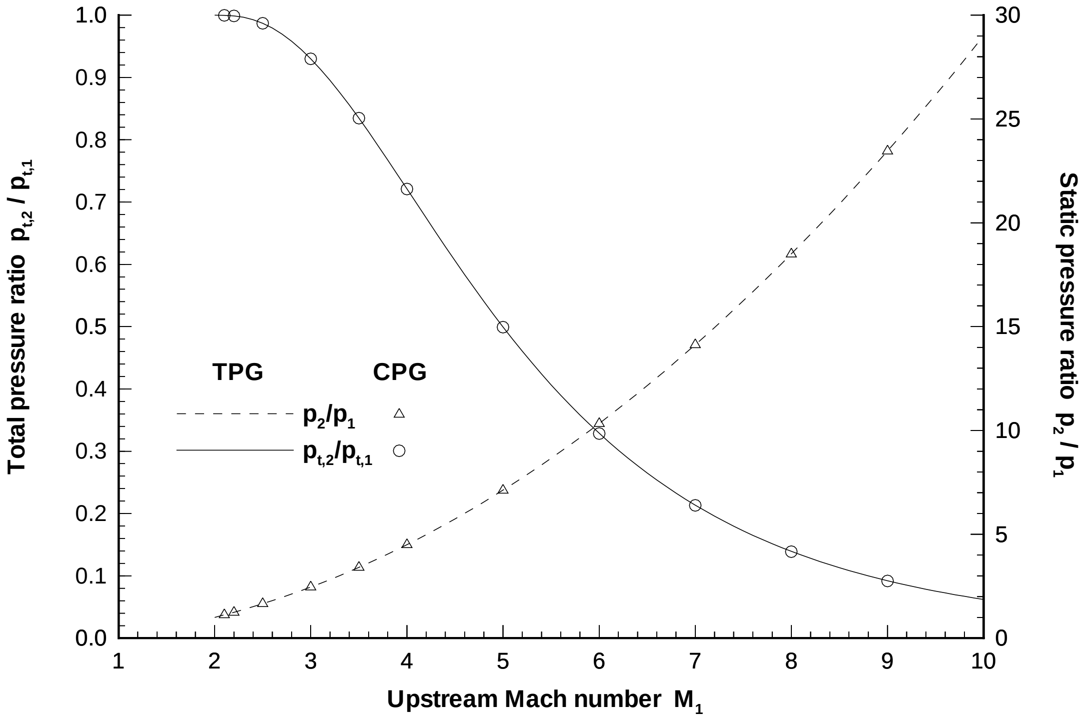


(a) Downstream Mach number M_2 and flow deflection angle δ



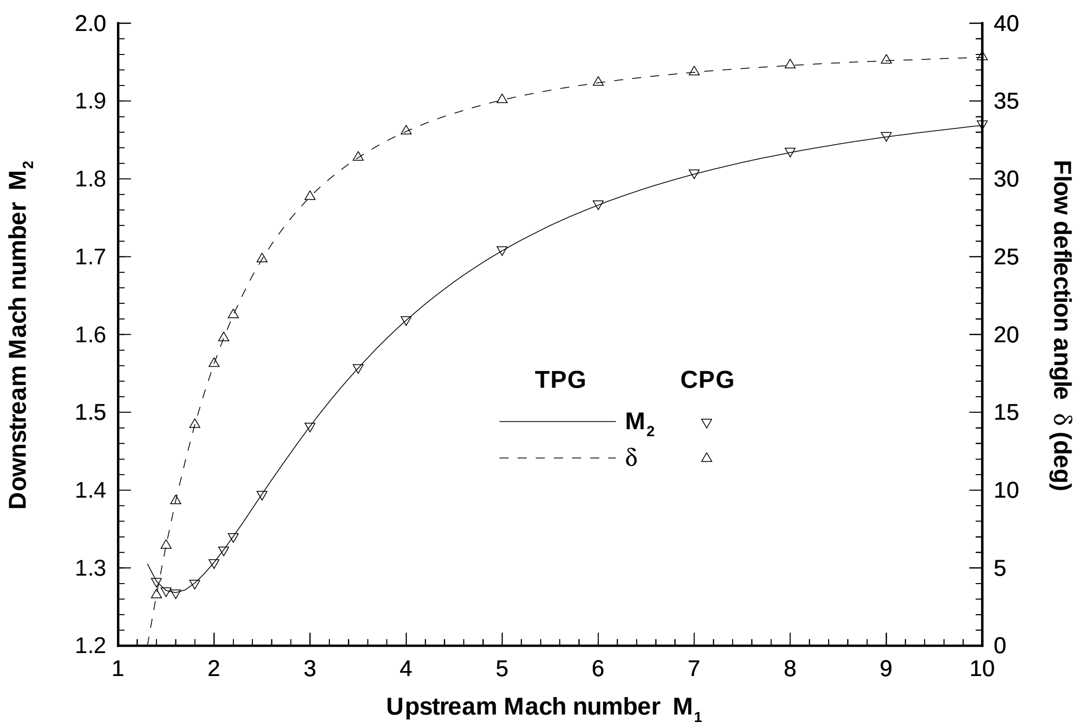
(b) Density ratio ρ_2/ρ_1 and temperature ratio T_2/T_1

Figure 3. Thermally and calorically perfect calculations of oblique shock wave properties within the calorically perfect temperature regime: air, T_t=400 K, σ=30°.



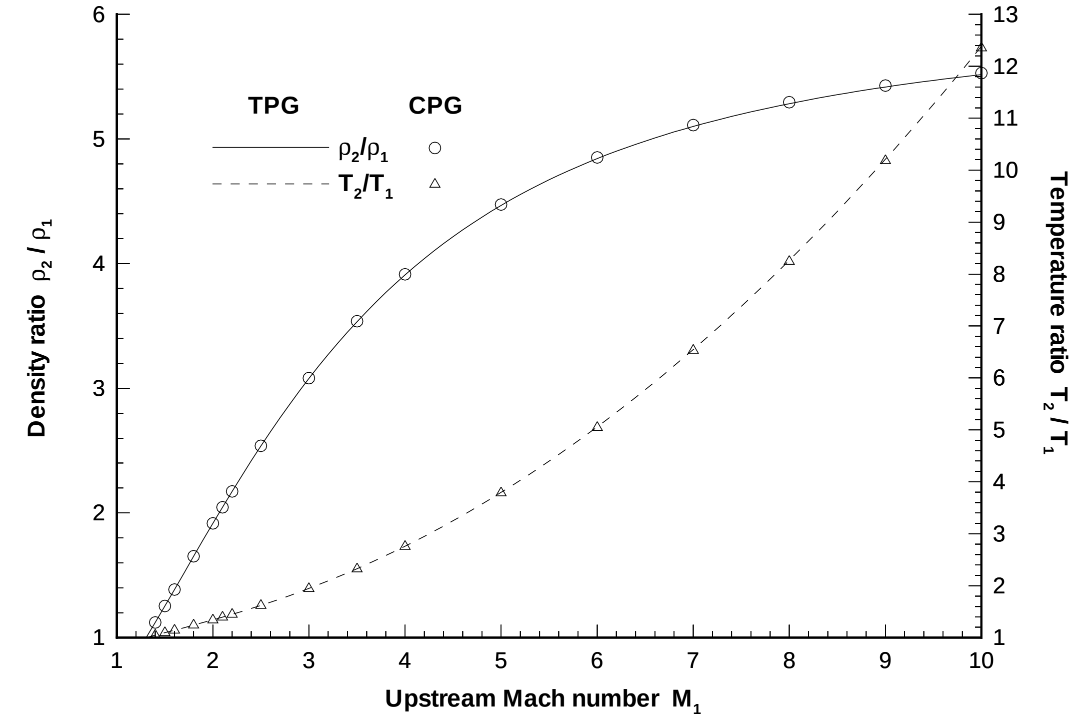
(c) Total and static pressure ratios $p_{t,2}/p_{t,1}$ and p_2/p_1

Figure 3. *Concluded*.

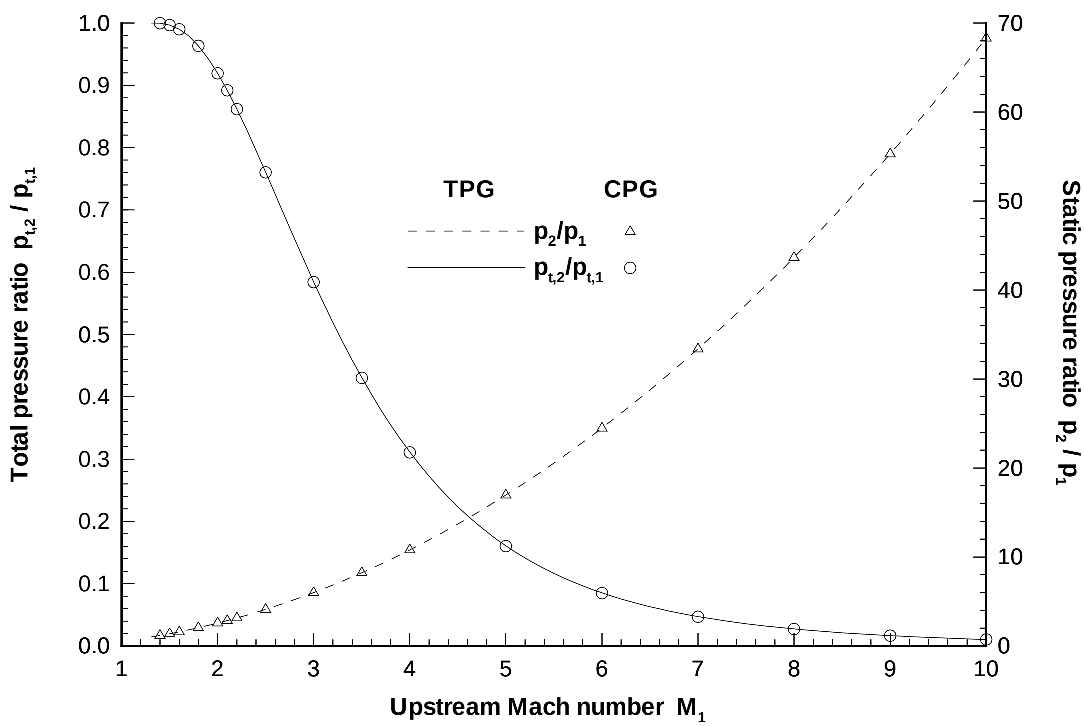


(a) Downstream Mach number M_2 and flow deflection angle δ

Figure 4. Thermally and calorically perfect calculations of oblique shock wave properties within the calorically perfect temperature regime: air, T_t=400 K, σ=50°.



(b) Density ratio ρ_2/ρ_1 and temperature ratio T_2/T_1



(c) Total and static pressure ratios $p_{t,2}/p_{t,1}$ and p_2/p_1

Figure 4. *Concluded*.

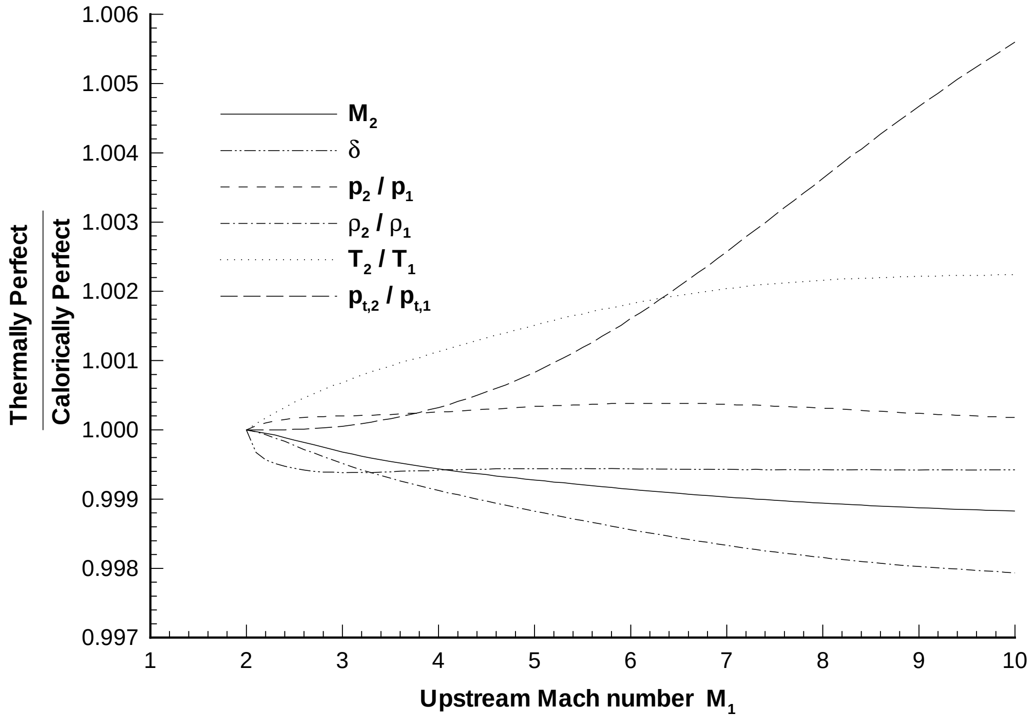


Figure 5. Effect of caloric imperfections on oblique shock wave properties within the calorically perfect temperature regime: air, T_t=400 K, σ=30°.

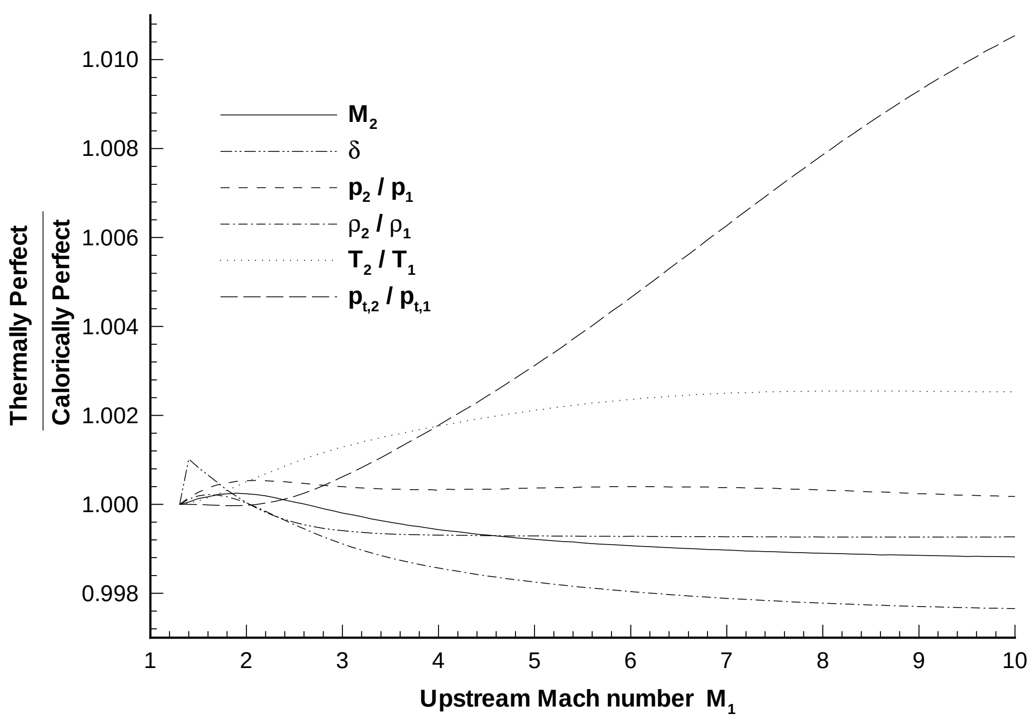
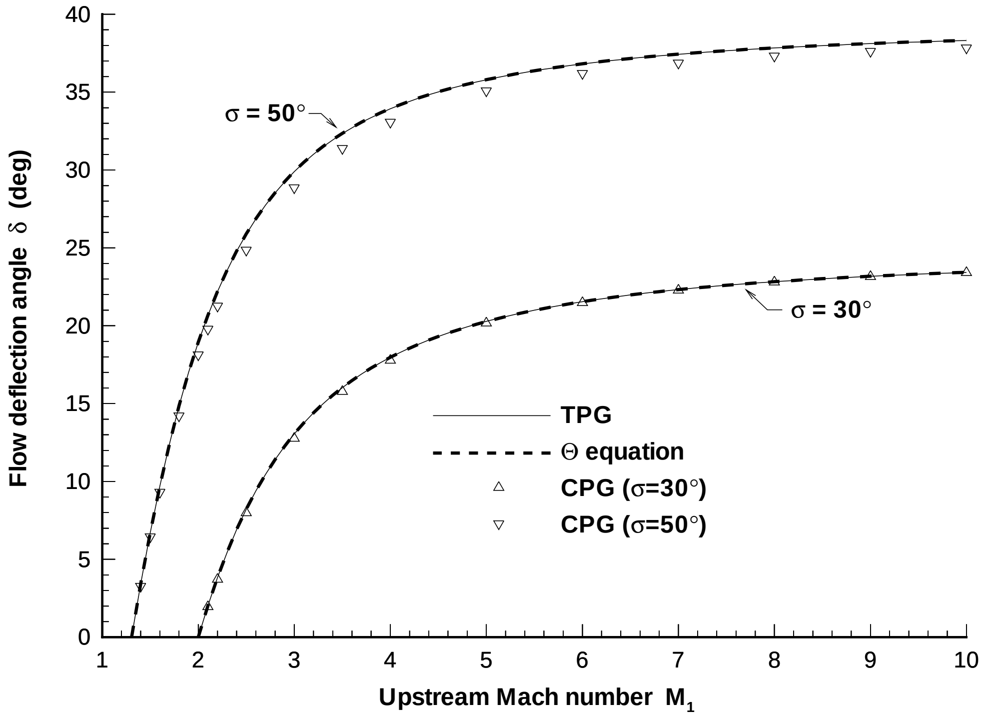
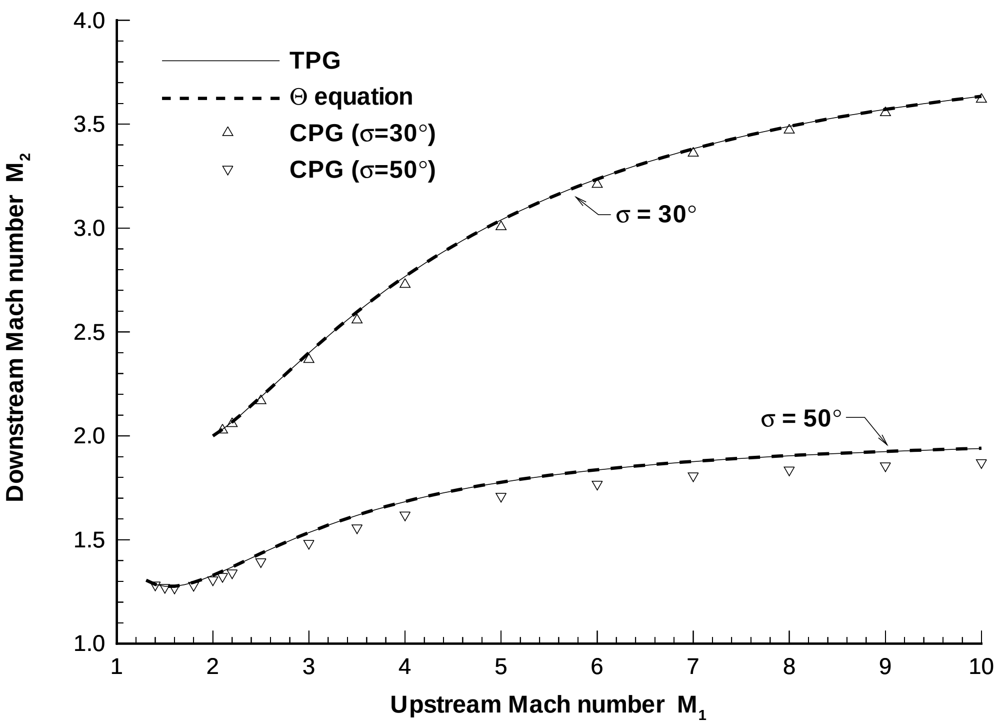


Figure 6. Effect of caloric imperfections on oblique shock wave properties within the calorically perfect temperature regime: air, T_t=400 K, σ=50°.

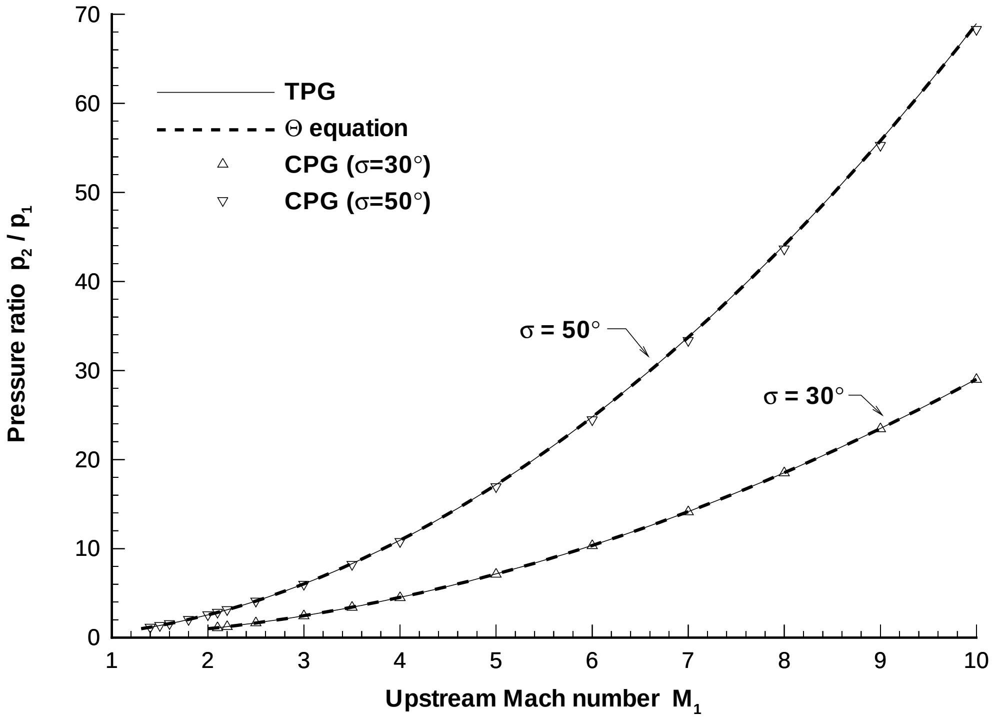


(a) Flow deflection angle δ

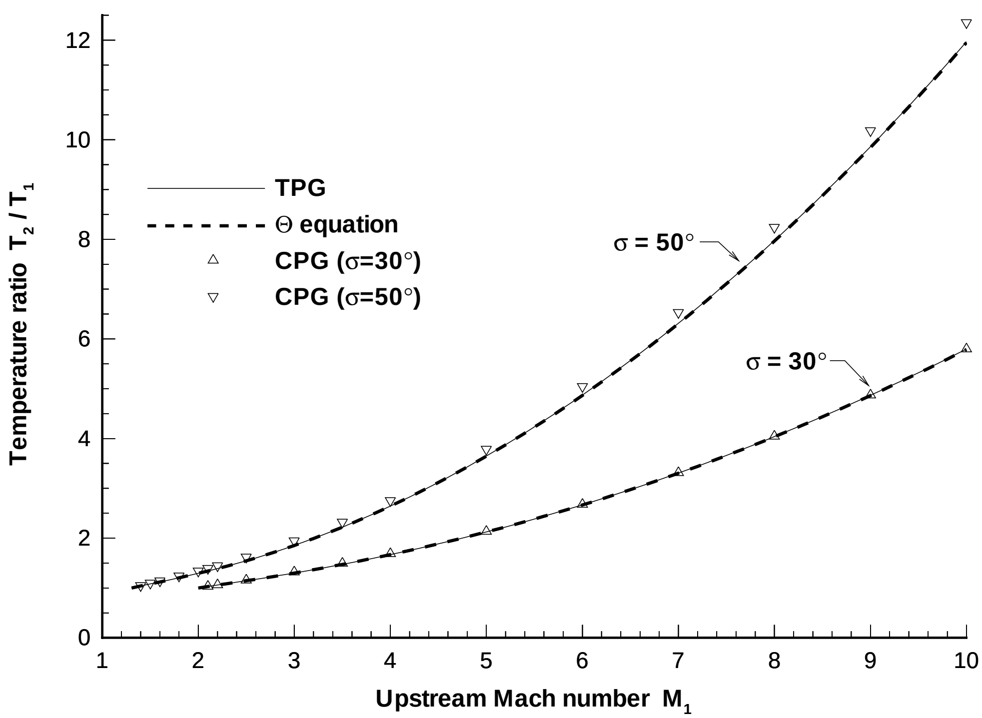


(b) Downstream Mach number M_2

Figure 7. Comparison of thermally and calorically perfect calculations for oblique shock waves in air at T_t=1500 K for σ=30° and 50°.

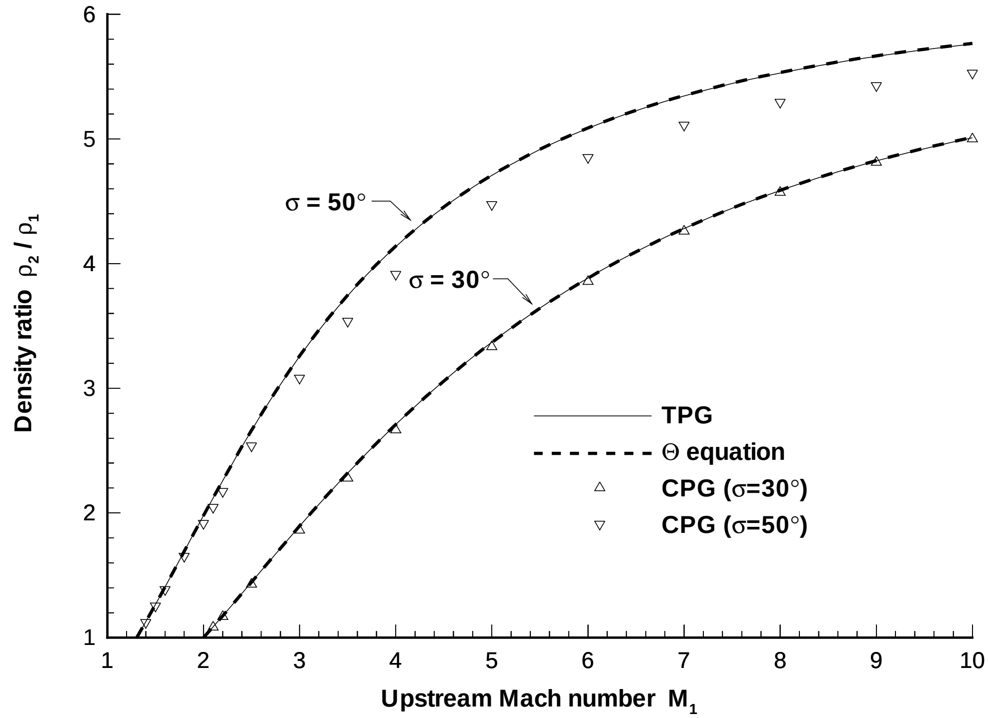


(c) Static pressure ratio p_2/p_1

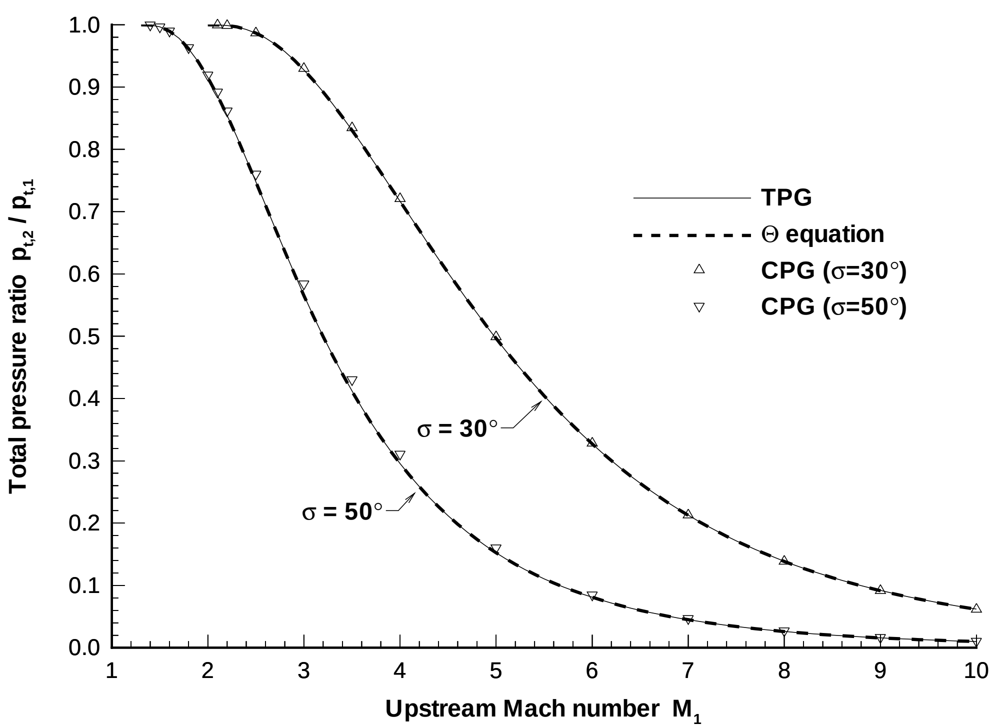


(d) Static temperature ratio T_2/T_1

Figure 7. *Continued*.

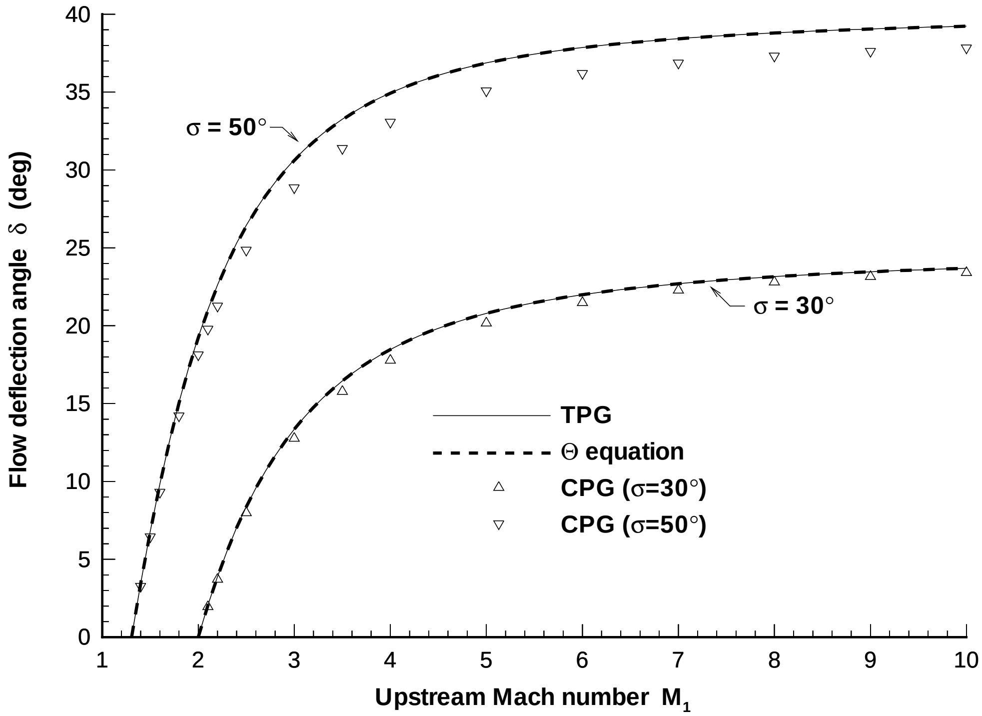


(e) Density ratio ρ_2/ρ_1

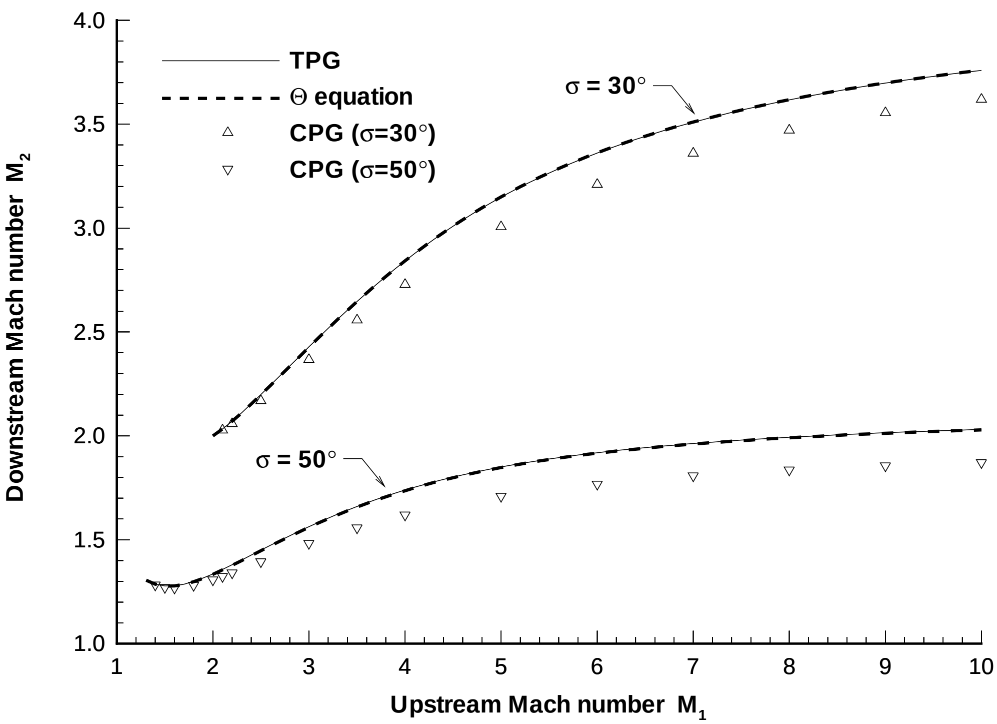


(f) Total pressure ratio $p_{t,2}/p_{t,1}$

Figure 7. *Concluded*.

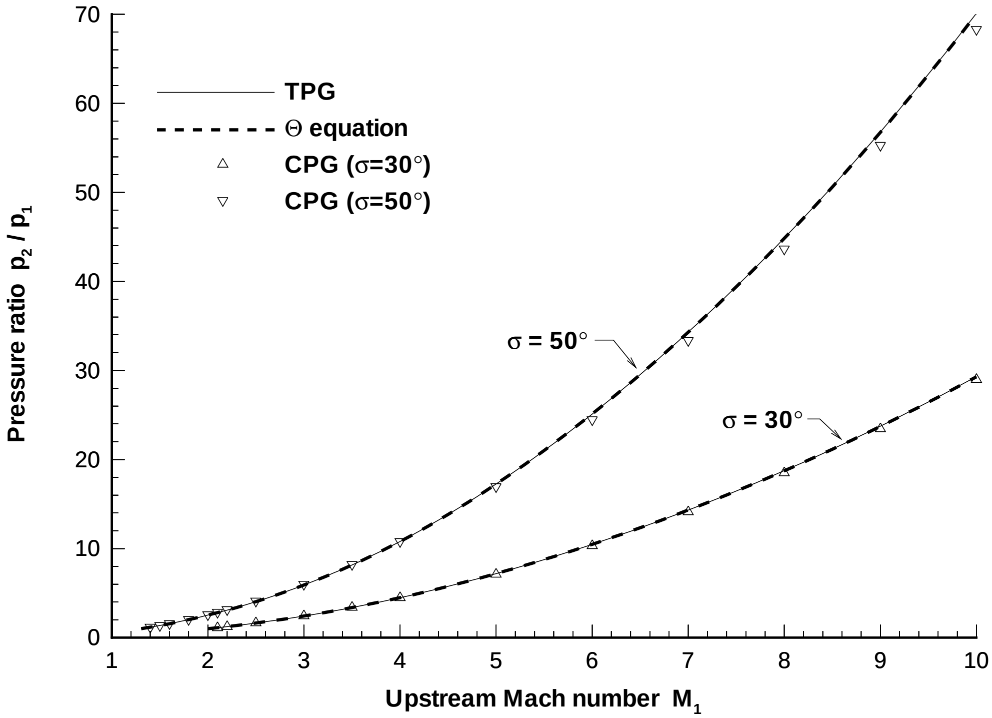


(a) Flow deflection angle δ

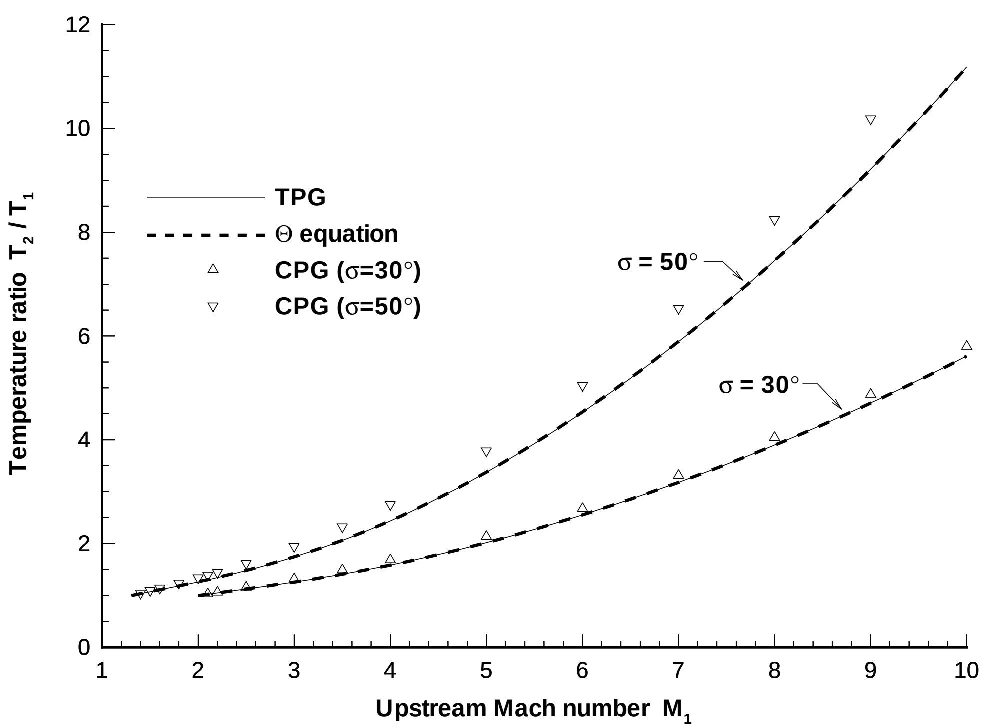


(b) Downstream Mach number M_2

Figure 8. Comparison of thermally and calorically perfect calculations for oblique shock waves in air at T_t=3000 K for σ=30° and 50°.

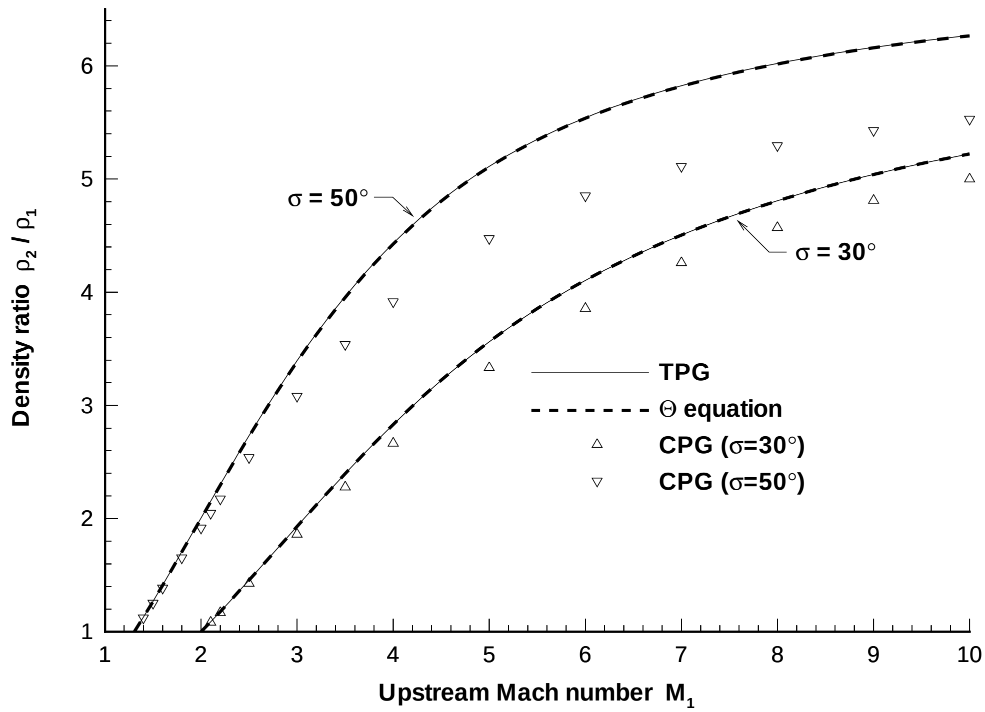


(c) Static pressure ratio p_2/p_1

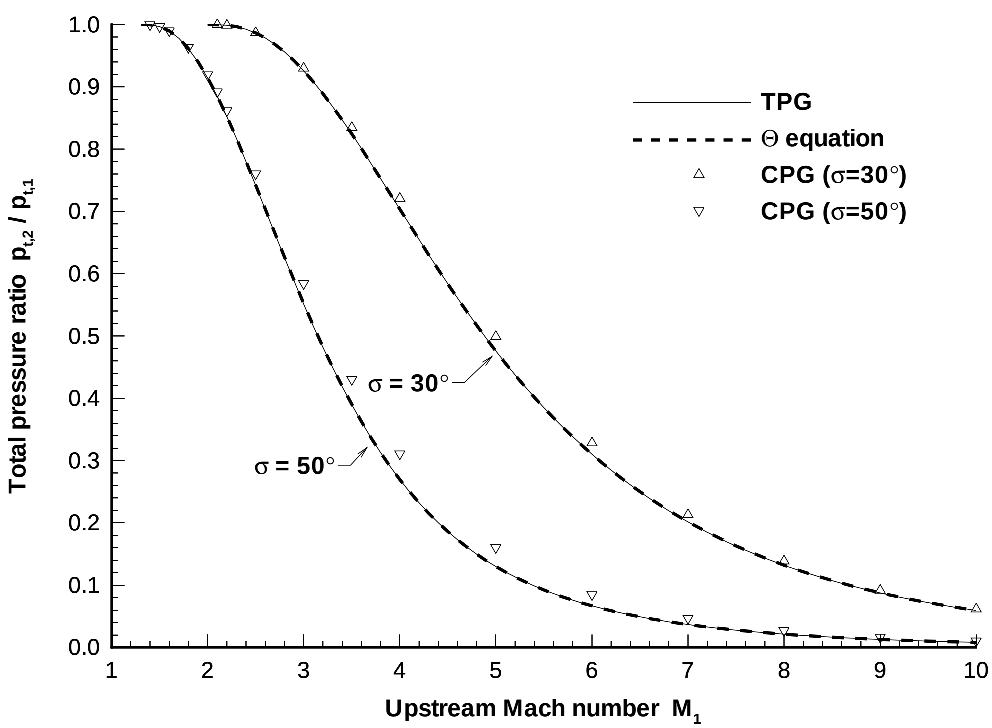


(d) Static temperature ratio T_2/T_1

Figure 8. *Continued*.

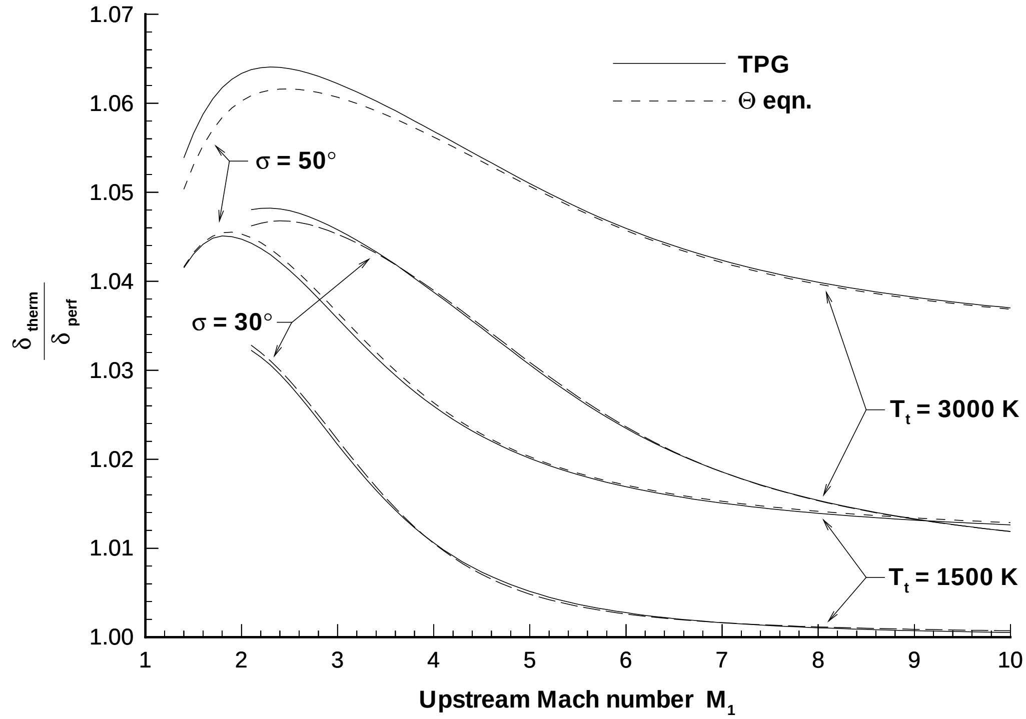


(e) Density ratio ρ_2/ρ_1

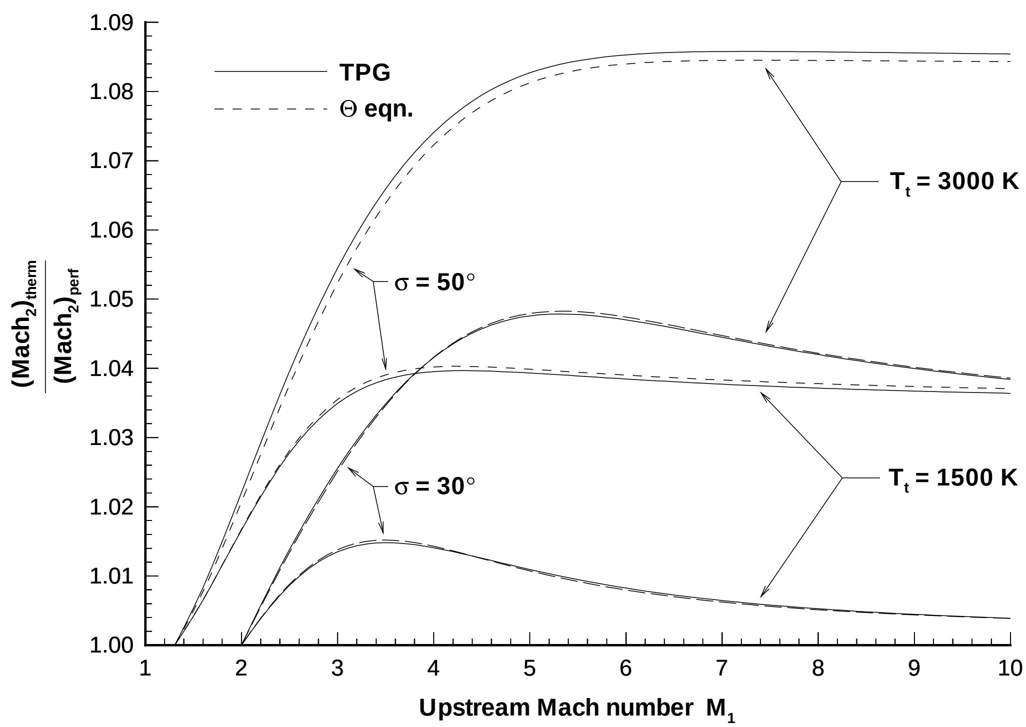


(f) Total pressure ratio $p_{t,2}/p_{t,1}$

Figure 8. *Concluded*.

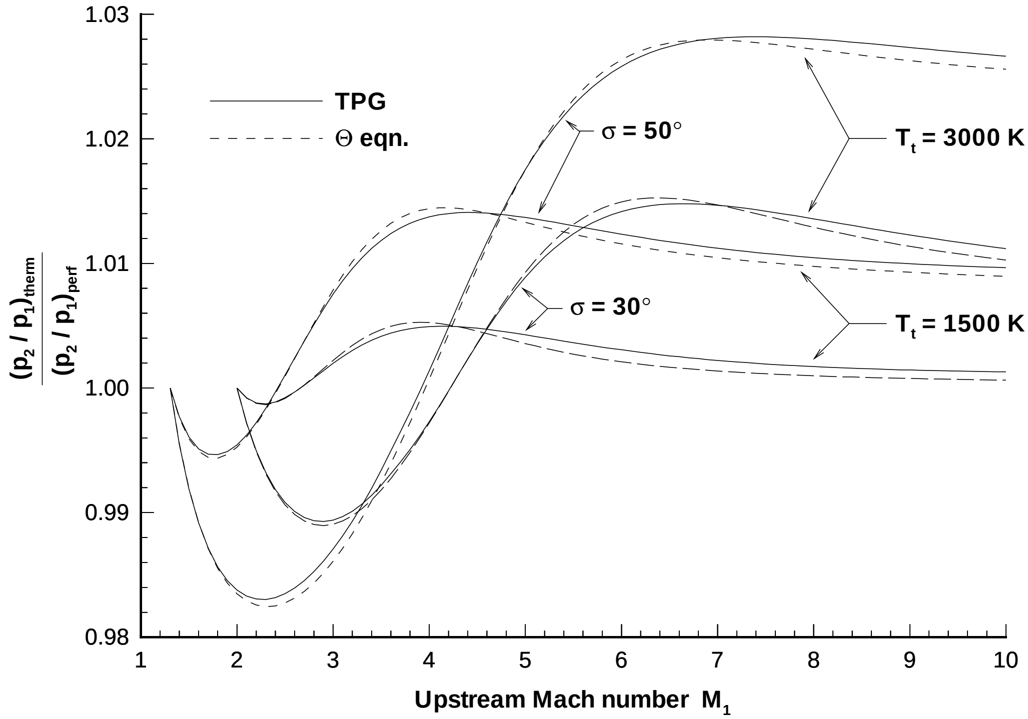


(a) Flow deflection angle δ

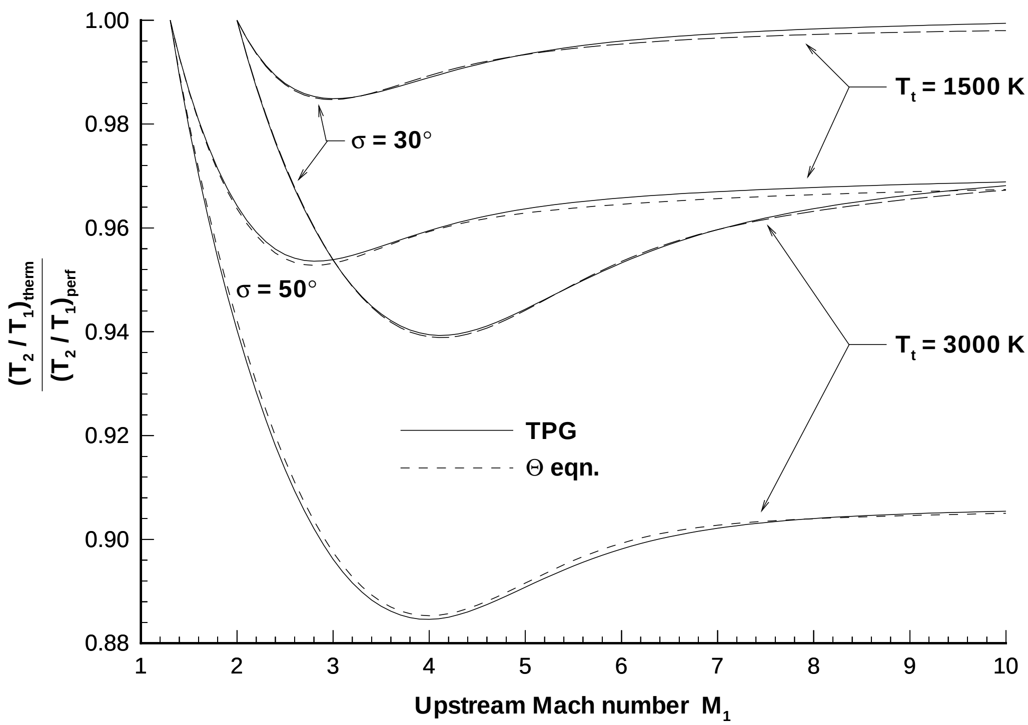


(b) Downstream Mach number M_2

Figure 9. Effect of caloric imperfections on oblique shock wave properties: comparisons between TPG and NACA Rep. 1135 for two total temperatures and two shock wave angles

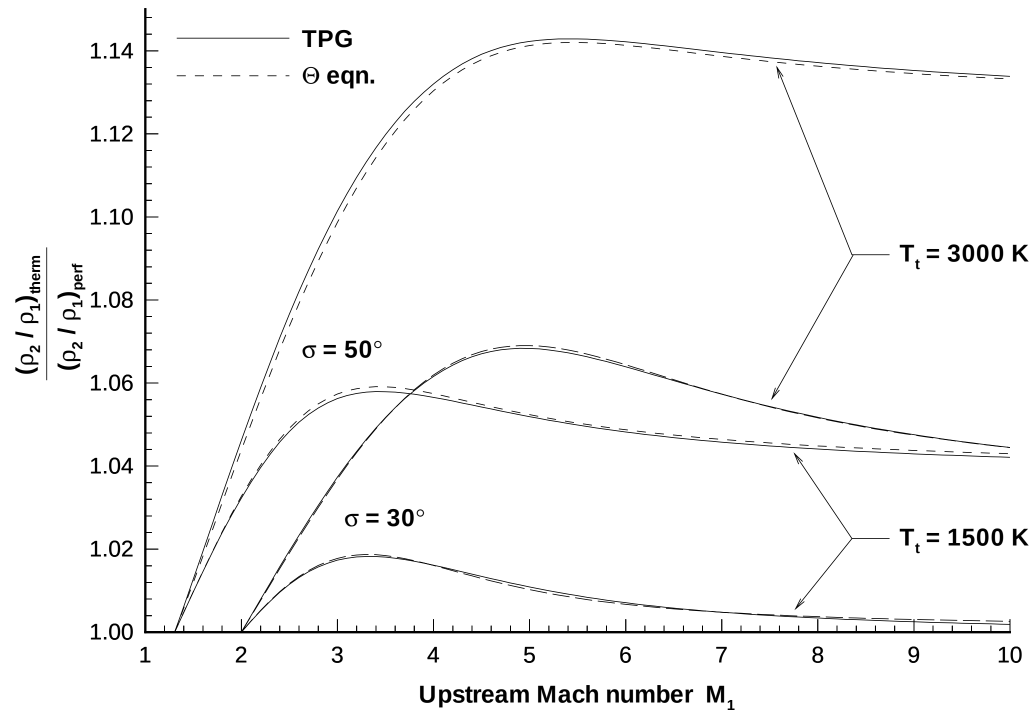


(c) Static pressure ratio p_2/p_1

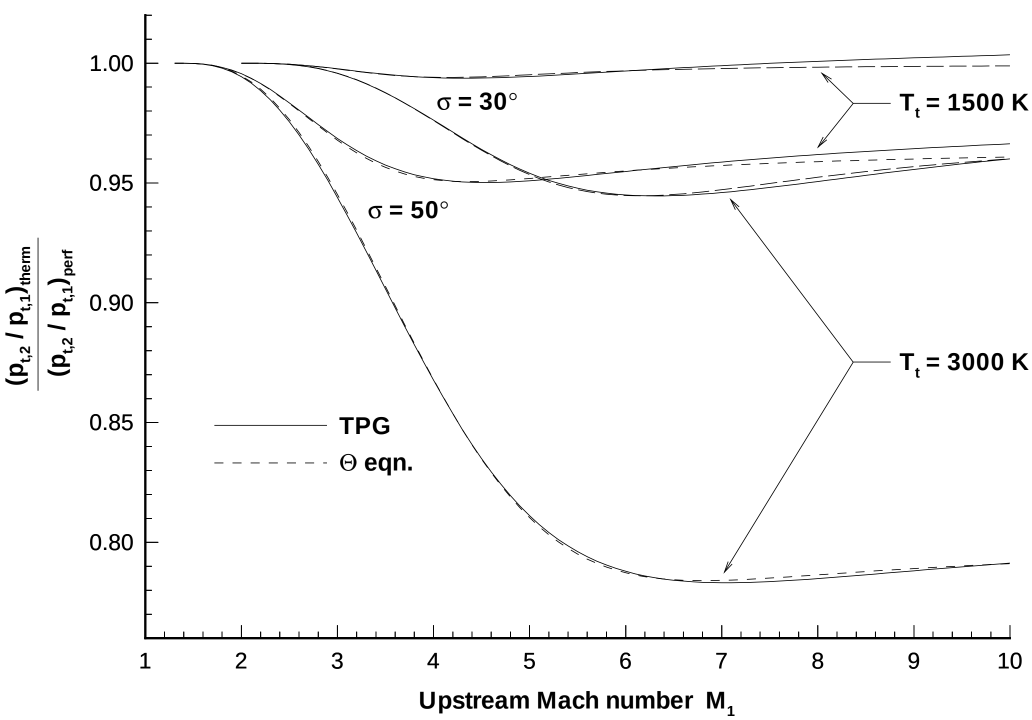


(d) Static temperature ratio T_2/T_1

Figure 9. *Continued*.



(e) Density ratio ρ_2/ρ_1



(f) Total pressure ratio $p_{t,2}/p_{t,1}$

Figure 9. *Concluded*.

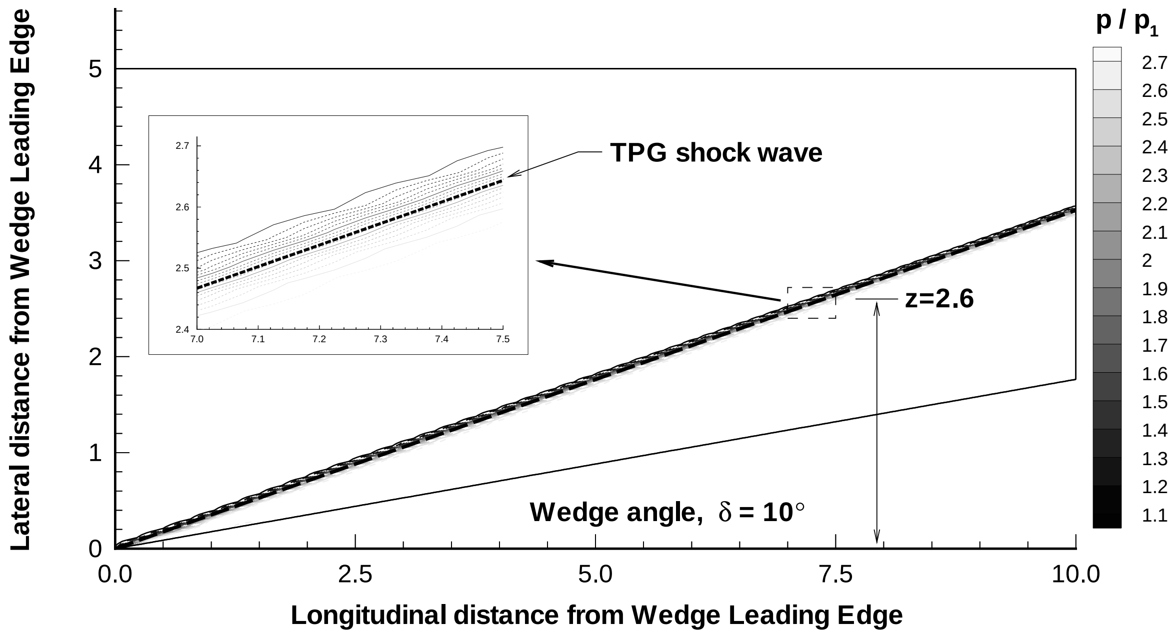
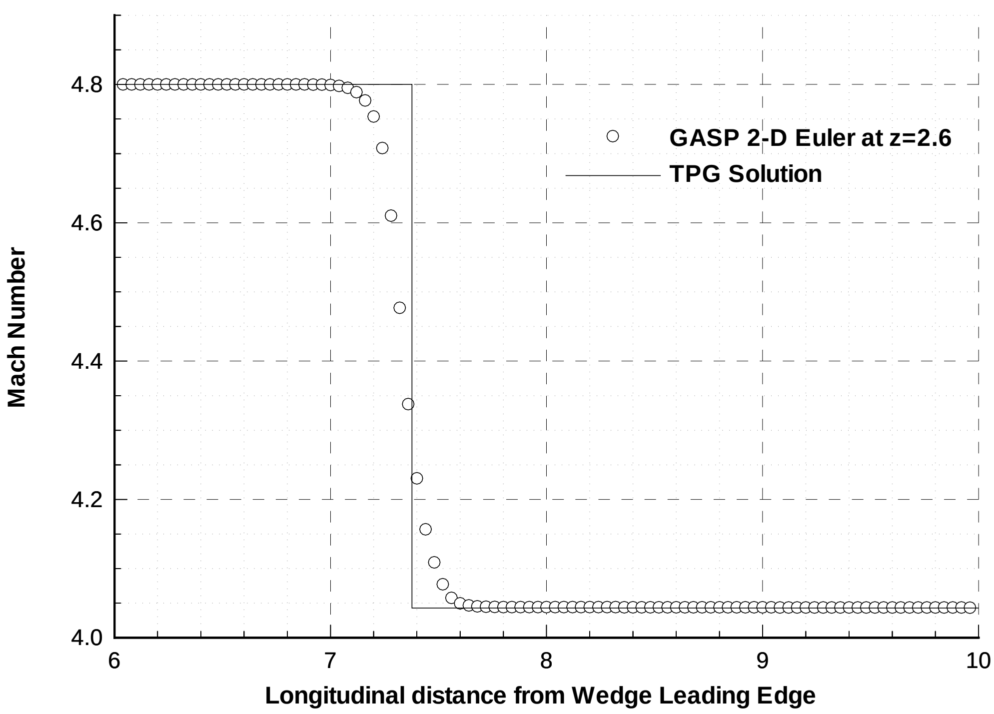
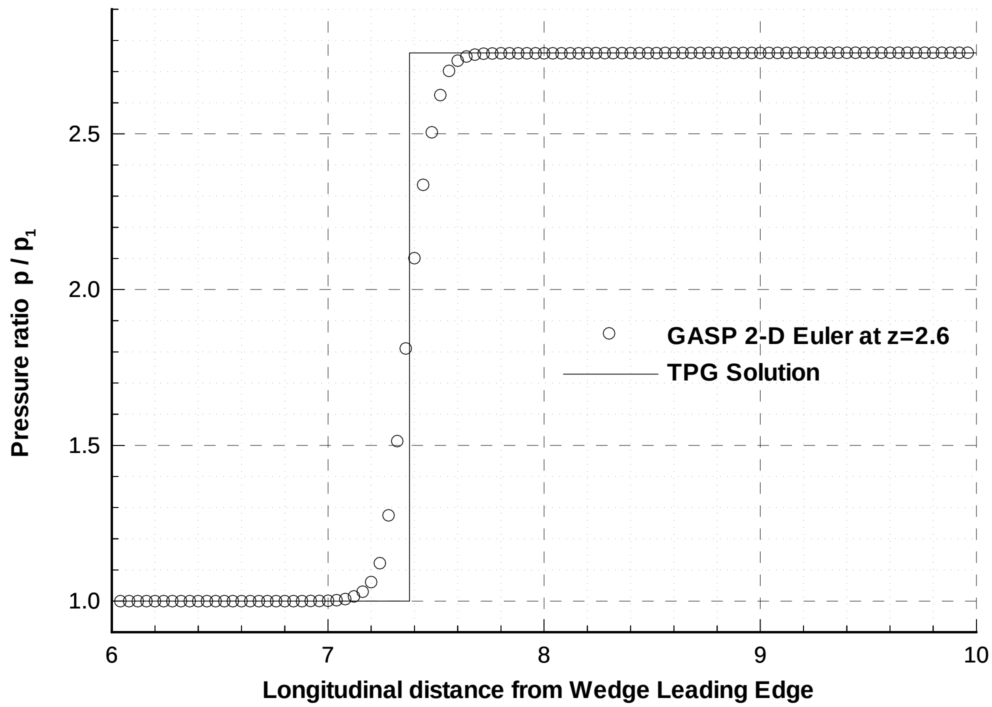


Figure 10. GASP 2-D Euler solution pressure ratio contours and TPG oblique shock wave for thermally perfect air: M_1=4.8, T_1=1670 K over a 10° wedge.

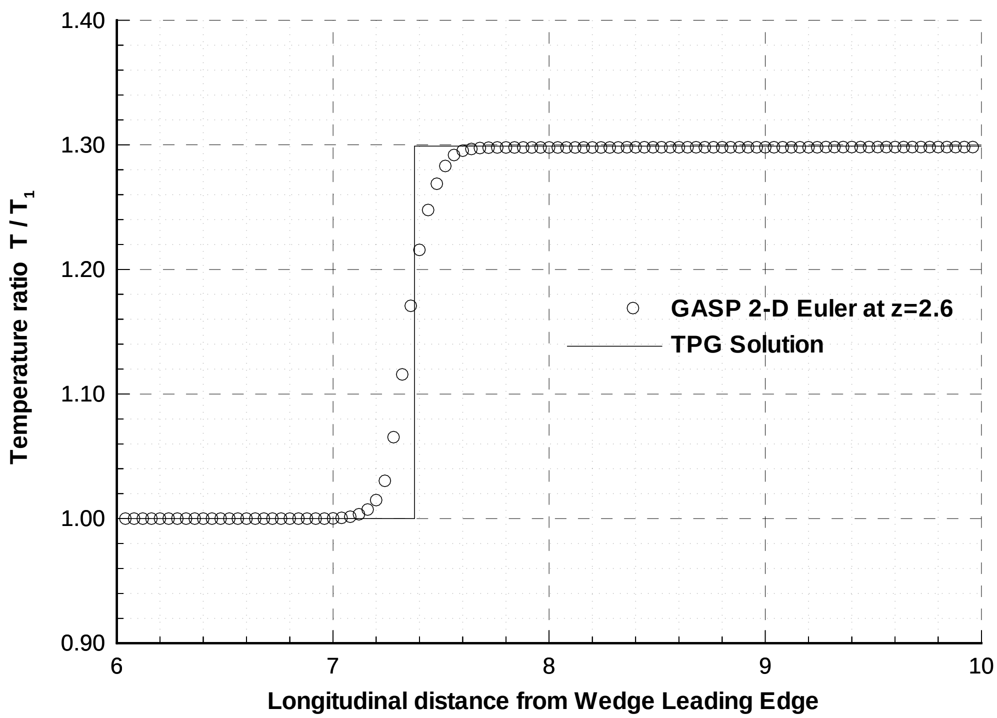


(a) Mach number M

Figure 11. GASP 2-D Euler and TPG oblique shock wave calculations for thermally perfect air: M_1=4.8, T_1=1670 K over a 10° wedge: at z=2.6 units above the wedge leading edge.

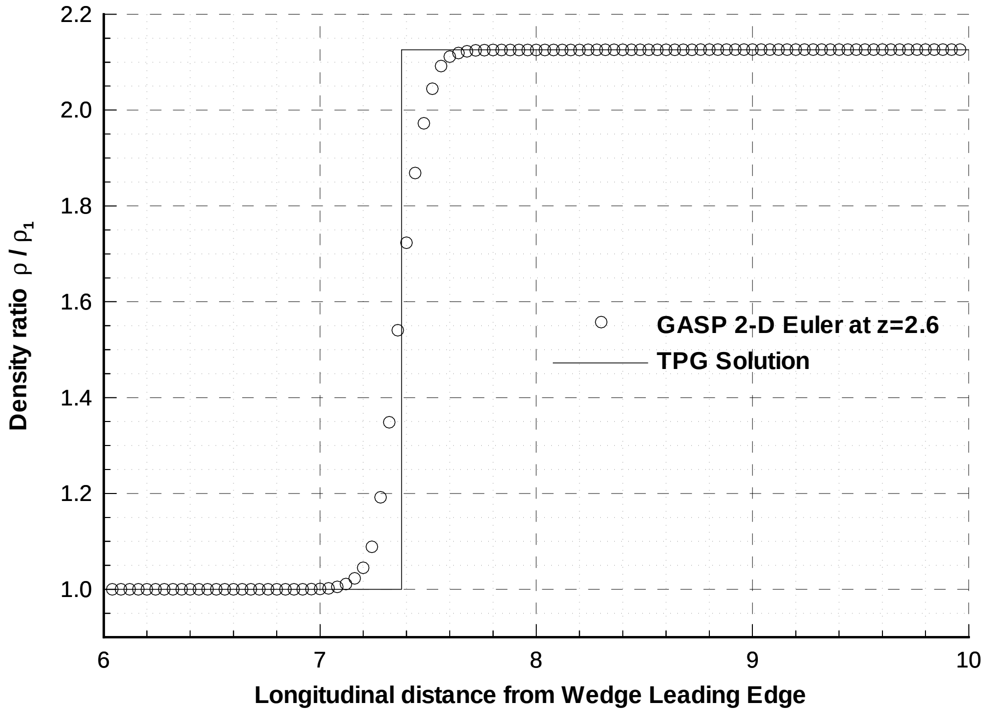


(b) Static pressure ratio p/p_1



(c) Static temperature ratio T/T_1

Figure 11. *Continued*.



(d) Density ratio ρ_2/ρ_1

Figure 11. *Concluded*.

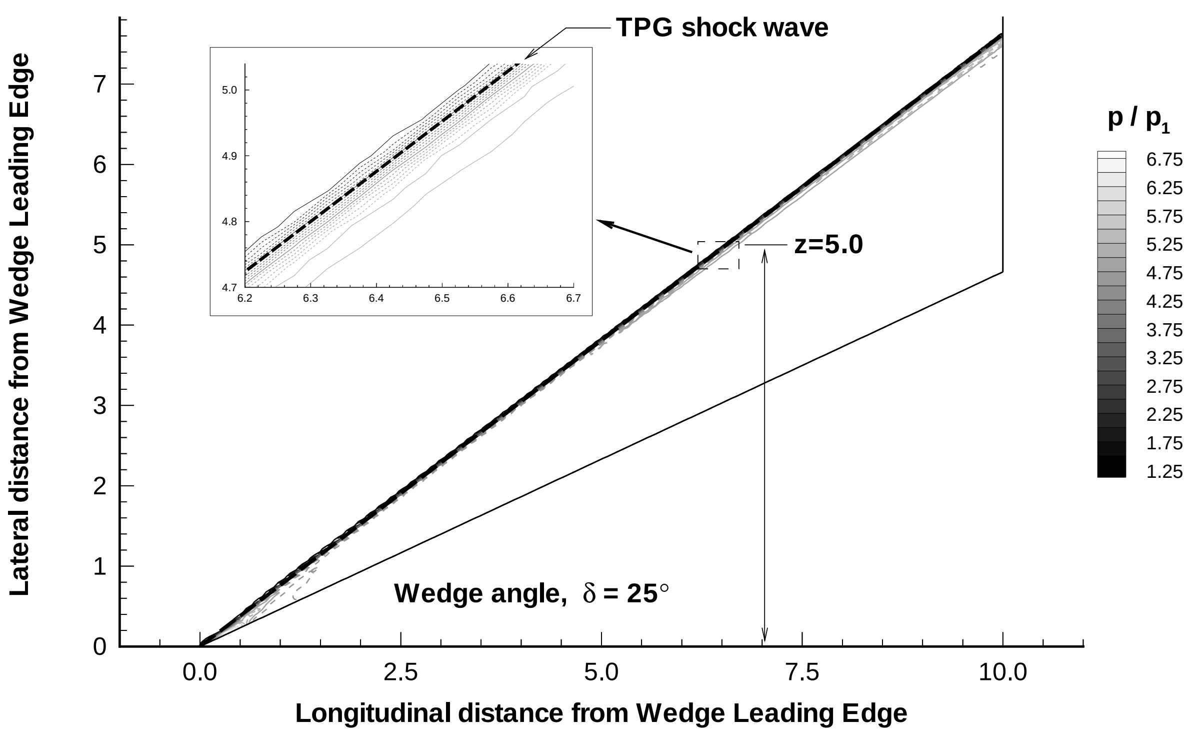
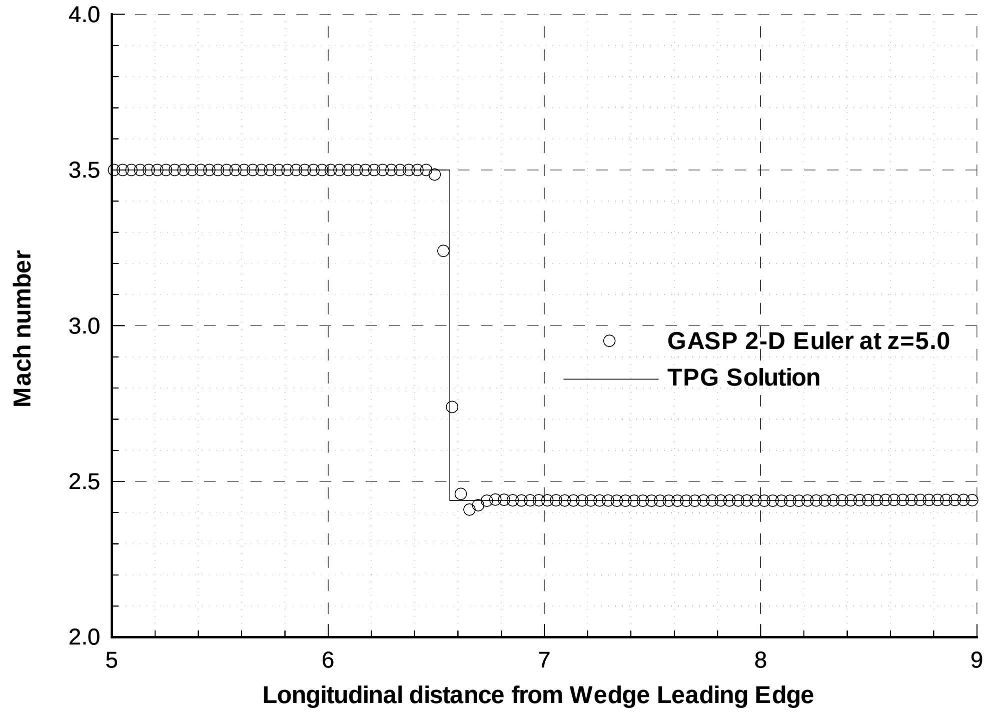
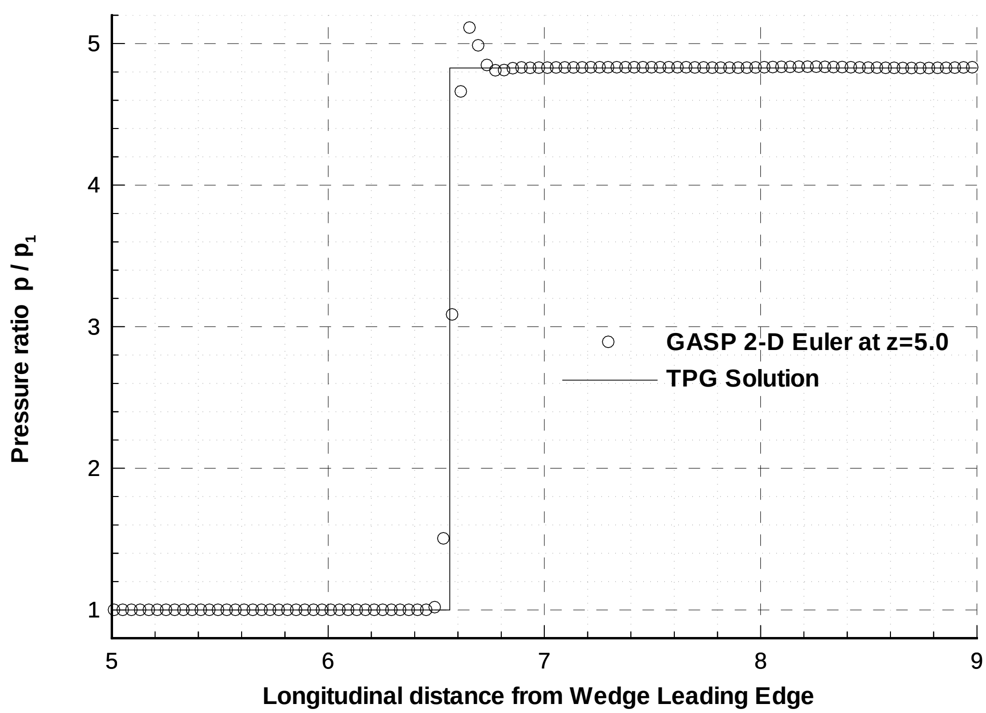


Figure 12. GASP 2-D Euler solution pressure ratio contours and TPG oblique shock wave for 20% Steam/80% CO_2, by mass: M_1=3.5, T_1=1200 K over a 25° wedge.

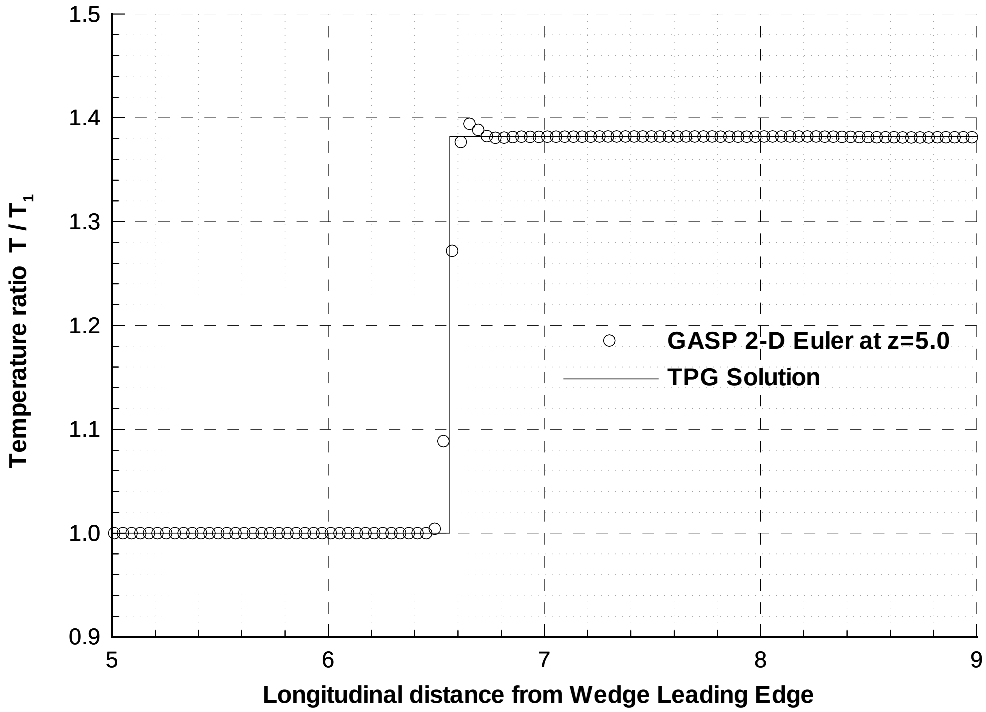


(a) Mach number M

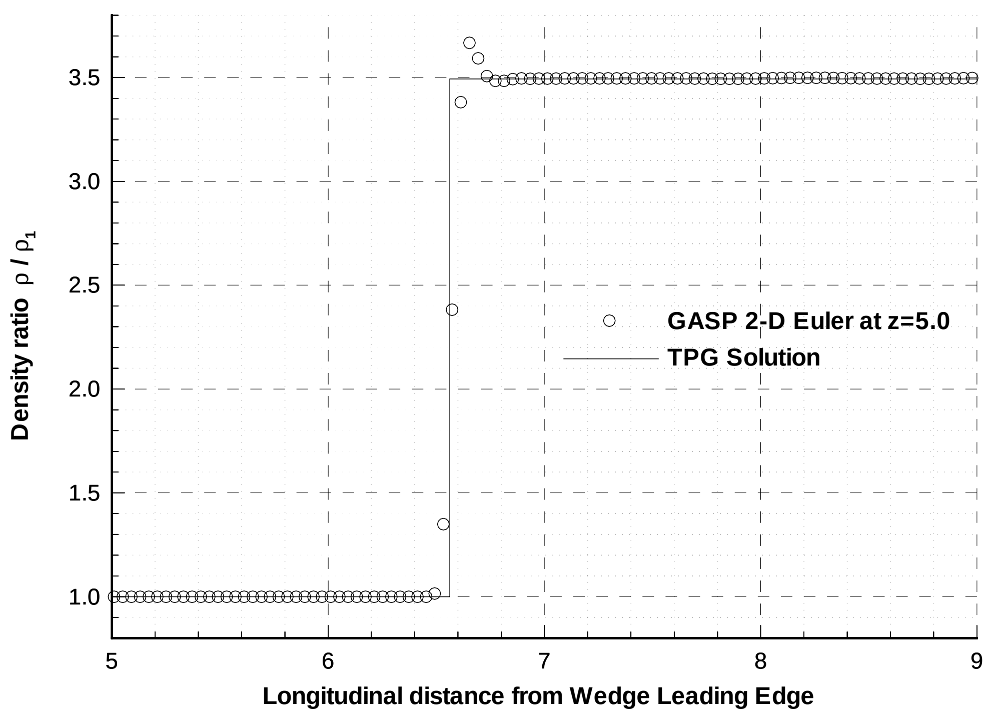


(b) Static pressure ratio p/p_1

Figure 13. GASP 2-D Euler and TPG oblique shock wave calculations for 20% Steam/80% CO_2, by mass: M_1=3.5, T_1=1200 K over a 25° wedge: at z=5.0 units above the wedge leading edge.



(c) Static temperature ratio T/T_1



(d) Density ratio ρ/ρ_1

Figure 13. *Concluded.*